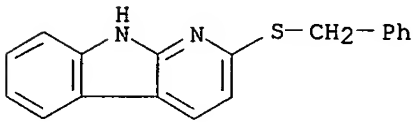
L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN **26148-35-6** REGISTRY
CN 9H-Pyrido[2,3-b]indole, 2-(benzylthio)- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H14 N2 S
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

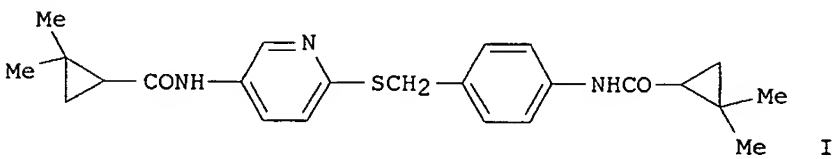
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

OK

AN 2001:31464 CAPLUS
DN 134:100762
ED Entered STN: 12 Jan 2001
TI Preparation of pyridine derivatives and medicinal use thereof
IN Iino, Yukio; Fujita, Kohichi; Kodaira, Ariko; Hatanaka, Toshihiro; Takehana, Kenji; Kobayashi, Tsuyoshi; Konishi, Atsushi; Yamamoto, Takashi
PA Ajinomoto Co., Inc., Japan
SO PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC C07D211-58; C07D213-75; C07D213-76; C07D237-20; C07D237-22; C07D239-42; C07D239-48; C07D277-44; A61K031-44; A61K031-445; A61K031-50; A61K031-505; A61P029-00
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002359	A1	20010111	WO 2000-JP4298	20000629
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1193255	A1	20020403	EP 2000-940879	20000629
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000012046	A	20020514	BR 2000-12046	20000629
	TW 519538	B	20030201	TW 2000-89113050	20000630
	US 2002133005	A1	20020919	US 2001-29871	20011231
PRAI	JP 1999-187959	A	19990701		
	JP 2000-71706	A	20000315		
	WO 2000-JP4298	W	20000629		

OS MARPAT 134:100762
GI



I

AB Heterocyclic compds. represented by the following general formula R1-CO-N(R2)-A-X-B-N(R3)-Y-(CH2)n-R4 [R1 = (un)substituted or cycloalkenyl; R2, R3 = H, alkyl; R4 = (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, or heterocyclyl having .gtoreq.1 heteroatom(s); A = (un)substituted heterocyclic ring; B = (un)substituted arom. or heterocyclic ring; n = 0-6; Y = a bond between atoms, CO, CO2, CONR5, C(S)NR5, SO, SO2 (wherein R5 = H, alkyl); X = a bond between atoms, O, OCHR7, CHR8O, O2C, CO2, OC(S), C(S)O, S, SO, SO2, SCHR9, CHR10S, SC(O), C(O)S, SC(S), C(S)S, SO2 NR11, NR12SO2, NR13, etc.; R7 - R10 = H, alkyl; R11 - R13 = H, alkyl, acyl] or pharmacol. acceptable salts thereof are

prepd. These compds. have inhibitory effects on AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor, etc. and are usable as drugs such as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics. Thus, 2-mercapto-5-nitropyridine was treated with NaH in DMF and then alkylated by 1-bromomethyl-4-nitrobenzene at room temp. for 1.5 h to give 2-(4-nitrobenzylthio)-5-nitropyridine which was reduced by Zn/AcOH in THF at room temp. for 16 h to 2-(4-aminobenzylthio)-5-aminopyridine and then acylated by 2,2-dimethylcyclopropanecarbonyl chloride in the presence of Et3N in CH2Cl2 at room temp. for 17 h to give 2-(4-(2,2-dimethylcyclopropanecarbonylamino)benzylthio)-5-(2,2-dimethylcyclopropanecarbonylamino)pyridine (I). I in vitro inhibited NF-kappa B activity with IC50 of 0.015 .mu.g/mL in an assay measuring .beta.-galactosidase activity expressed in HUVEC cells and driven by NF-kappa B-binding sequence-fused SV40 T antigen min. promoter.

ST pyridine prepn antiinflammatory; antirheumatic pyridine prepn; **antiviral** immunosuppressant pyridine prepn; cancer metastasis inhibitor pyridine prepn; antiarteriosclerotics pyridine prepn

IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(AP-1 (activator protein 1); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(NF-.kappa. B (nuclear factor .kappa. B); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cell adhesion
(factor, inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Antitumor agents
(metastasis; prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT Anti-inflammatory agents
Antiarteriosclerotics
Antirheumatic agents
Antiviral agents
Immunosuppressants
(prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT 318967-19-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 318967-14-5P 318967-15-6P 318967-16-7P 318967-17-8P 318967-18-9P
318967-20-3P 318967-21-4P 318967-22-5P 318967-23-6P 318967-24-7P
318967-25-8P 318967-26-9P **318967-27-0P** 318967-28-1P
318967-29-2P 318967-30-5P 318967-31-6P 318967-32-7P 318967-33-8P
318967-34-9P 318967-35-0P 318967-36-1P 318967-37-2P 318967-38-3P
318967-39-4P 318967-40-7P 318967-41-8P 318967-42-9P 318967-43-0P
318967-44-1P 318967-45-2P 318967-46-3P 318967-47-4P 318967-48-5P
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318967-54-3P 318967-55-4P 318967-56-5P 318967-57-6P 318967-58-7P
318967-59-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 81669-70-7, Metalloprotease
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 88-75-5, 2-Nitrophenol 98-09-9, Benzenesulfonyl chloride 98-88-4, Benzoyl chloride 100-02-7, 4-Nitrophenol, reactions 100-11-8, 4-Nitrobenzyl bromide 103-63-9, 2-Bromoethylbenzene 103-71-9, Phenyl isocyanate, reactions 103-72-0, Phenyl isothiocyanate 103-80-0, Phenylacetyl chloride 104-03-0, 4-Nitrophenylacetic acid 108-24-7, Acetic anhydride 122-04-3, 4-Nitrobenzoyl chloride 123-30-8, 4-Hydroxyaniline 554-84-7, 3-Nitrophenol 636-98-6, 1-Iodo-4-nitrobenzene 637-59-2, 3-Phenylpropyl bromide 661-69-8, Hexamethylditin 932-67-2, 3-Cyclohexenecarbonyl chloride 1821-12-1, 4-Phenylbutanoic acid 1849-36-1, 4-Nitrobenzenethiol 2127-09-5, 2-Mercapto-5-nitropyridine 2581-34-2, 3-Methyl-4-nitrophenol 2719-27-9, Cyclohexanecarbonyl chloride 3073-77-6, 2-Amino-5-nitropyrimidine 3958-57-4, 3-Nitrobenzyl bromide 3958-60-9, 2-Nitrobenzyl bromide 4487-59-6, 2-Bromo-5-nitropyridine 4548-45-2, 2-Chloro-5-nitropyridine 4693-91-8, 4-Methoxyphenylacetyl chloride 5339-26-4, 2-(4-Nitrophenyl)ethyl bromide 5365-15-1, 2,2-Dichlorocyclopropanecarbonyl chloride 5418-51-9, 2-Hydroxy-5-nitropyridine 5469-69-2, 3-Amino-6-chloropyridazine 7169-97-3, 2-Acetamido-5-bromopyridine 10313-60-7, 3,4-Dimethoxyphenylacetyl chloride 14221-01-3, Tetrakis(triphenylphosphine)palladium 23056-33-9, 2-Chloro-4-methyl-5-nitropyridine 24424-99-5, Di-tert-butyl dicarbonate 25026-34-0, 4-Chlorophenylacetyl chloride 33332-29-5 39053-78-6, 3,4,5-Trimethoxyphenylacetyl chloride 50541-93-0, 4-Amino-1-benzylpiperidine 50675-57-5, 2,2-Dimethylcyclopropanecarbonyl chloride 54840-15-2, 4-(tert-Butoxycarbonylamino)phenol 55972-71-9, p-Phenylenediamine hydrochloride 60733-34-8, 2-Methylcyclopropanecarbonyl chloride 69097-20-7, Tris(trimethylsiloxy)ethylene 89312-77-6 90403-98-8, 2-Methylcyclohexanecarbonyl chloride 103554-20-7 193204-58-9 318967-66-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 4982-09-6P 13534-97-9P, 5-Amino-2-bromopyridine 24253-19-8P
29958-19-8P 32605-02-0P 34295-27-7P 99844-01-6P 109899-69-6P
116735-74-1P 318967-60-1P 318967-61-2P 318967-62-3P 318967-63-4P

318967-64-5P 318967-65-6P 318967-67-8P 318967-68-9P 318967-69-0P
318967-70-3P 318967-71-4P 318967-72-5P 318967-73-6P 318967-74-7P
318967-75-8P 318967-76-9P **318967-77-0P 318967-78-1P**
318967-79-2P 318967-80-5P 318967-81-6P 318967-82-7P 318967-83-8P
318967-84-9P 318967-85-0P 319459-36-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Ajinomoto Co Inc; WO 200015603 A1 2000
(2) Boehringer Ingelheim Pharmaceuticals Inc; JP 2000502702 A
(3) Boehringer Ingelheim Pharmaceuticals Inc; US 6057451 A CAPLUS
(4) Boehringer Ingelheim Pharmaceuticals Inc; WO 9724343 A1 1997 CAPLUS
(5) Smithkline Beecham Corp; JP 2000500464 A
(6) Smithkline Beecham Corp; JP 2000500464 A
(7) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
(8) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
(9) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS
(10) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS

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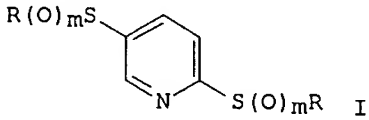
OK

AN 1987:32855 CAPLUS
DN 106:32855
ED Entered STN: 07 Feb 1987
TI 2,5-Bis(alkylsulfonyl)- and 2,5-bis(alkylthio)-substituted-pyridines
IN Wood, Steven G.
PA Dow Chemical Co., USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D211-72
ICS C07D211-84
NCL 546294000
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4616087	A	19861007	US 1982-380642	19820521

PRAI US 1982-380642 19820521
OS CASREACT 106:32855
GI



I

AB The title compds. I (R = C1-7 alkyl, cycloalkyl, Ar(CH2)q, Ar = (un)substituted Ph, naphthyl; q = 0-3; m = 0-2) useful as **antiviral** agents, were prepd. Thus, to 4-F3CSC6H4OH in THF was added Me3COK and 2,5-bis(methylsulfonyl)pyridine, prepd. in 3 steps from Me 3,6-dichloro-2-pyridinecarboxylate, to give 5-(methylsulfonyl)-2-[4-[(trifluoromethyl)thio]phenoxy]pyridine (II). II at 12.5 .mu.g/mL was active against rhinovirus type 1A.

ST pyridine alkylsulfonyl phenoxy prepn **antiviral**

IT Virucides and Virustats
(bis(alkylsulfonyl)- and bis(alkylthio)-substituted-pyridines)

IT 533-31-3, 3,4-(Methylenedioxy)phenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bis(ethylsulfonyl)pyridine)

IT 106-41-2, 4-Bromophenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bis(hexylsulfonyl)pyridine)

IT 461-84-7, 4-(Trifluoromethylthio)phenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bis(methylsulfonyl)pyridine)

IT 95-77-2, 3,4-Dichlorophenol 99-93-4, p-Hydroxyacetophenone 1137-42-4, p-Hydroxybenzophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with sulfonylpyridines)

IT 85330-64-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with (methylenedioxy)phenol)

IT 85330-63-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with (trifluoromethylthio)phenol)

IT 85330-69-4P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and condensation with bromophenol)

IT 85330-66-1P 85330-75-2P 85330-79-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with dichlorophenol)

IT 85330-72-9P 85330-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with hydroxyacetophenone)

IT **85330-78-5P** 85330-89-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with hydroxybenzophenone)

IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**
85331-32-4P 91164-62-4P 106025-37-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation of)

IT 85331-31-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation-oxidn. of)

IT 69212-36-8P 85330-62-7P 85330-65-0P 85330-68-3P 85330-71-8P
85330-74-1P **85330-77-4P** 85330-80-9P 85330-81-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

IT 98626-97-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P
85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P 85330-96-7P
85330-97-8P 85330-98-9P 85330-99-0P 85331-02-8P 85331-03-9P
85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P
85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P
85331-14-2P 85331-15-3P 85331-16-4P 85331-17-5P 85331-18-6P
85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P 85345-64-8P
85368-98-5P 99902-97-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as virucide)

IT 74-93-1, reactions 75-33-2 111-31-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution by, of Me dichloropyridinecarboxylate)

IT 75-08-1 100-53-8, Benzyl mercaptan 108-98-5, Thiophenol, reactions
1569-69-3, Cyclohexyl mercaptan
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution by, of dichloropyridinecarboxylic acid)

IT 1702-17-6, 3,6-Dichloro-2-pyridinecarboxylic acid 88912-24-7,
5,6-Dichloro-2-pyridinecarboxylic acid
RL: PROC (Process)
(substitution of, with mercaptans)

IT 1532-24-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution with alkanethiol and hydrolysis of)

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AN 1996:155490 CAPLUS
DN 124:202255
ED Entered STN: 19 Mar 1996
TI Preparation of sulfur-containing heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents
IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.
PA G. D. Searle and Co., USA
SO PCT Int. Appl., 212 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D235-28
ICS A61K031-415; C07D401-12; A61K031-44; C07D233-84
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523950	A1	19951129	AU 1995-23950	19950501
	US 5945425	A	19990831	US 1996-737251	19961024
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	A2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		
	US 2000-605560	B1	20000627		

OS MARPAT 124:202255
AB The title compds., which are (H+/K+) ATPase inhibitors, useful for the treatment of viral infections, are prepd. and formulations contg. them are claimed. Thus, 2-[(1H-benzimidazol-2-yl)sulfinylmethyl]-N,N-dimethylbenzenamine, m.p. 107-109.degree., was prepd. and demonstrated a (H+/K+) ATPase IC50 of 0.7 .mu.M.
ST benzimidazolylsulfinylmethylmethylbenzenamine prepn ATPase inhibitor; **antiviral** agent prepn benzimidazolylsulfinylmethylmethylbenzenamin e; benzimidazolyl sulfinylmethylmethylbenzenamine
IT Ulcer inhibitors
Virucides and Virustats
(heterocyclic (H+/K+) ATPase inhibitors)
IT 9000-83-3, ATPase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(potassium-hydrogen-activated; prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)
IT 55546-06-0P 56713-45-2P 57235-18-4P 60524-97-2P 71670-48-9P
73590-36-0P 73590-58-6P 73590-61-1P 81527-04-0P 81864-40-6P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 125214-42-8P 126026-46-8P 128429-74-3P 128935-96-6P 128936-05-0P
130049-59-1P 130368-60-4P 130368-62-6P 130368-66-0P 133903-90-9P
134017-66-6P 134462-81-0P 135430-38-5P 135461-65-3P 135863-25-1P
137105-02-3P 137247-56-4P 137810-46-9P 139644-93-2P 139767-99-0P
142062-72-4P 150064-18-9P 150460-06-3P 153284-85-6P 174397-92-3P
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174398-03-9P 174398-04-0P **174398-05-1P** 174398-06-2P
174398-07-3P 174398-08-4P 174398-09-5P 174398-10-8P 174398-11-9P
174398-12-0P 174398-13-1P 174398-14-2P 174398-15-3P 174398-16-4P
174398-17-5P 174398-18-6P 174398-19-7P 174398-20-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 144114-21-6, Retropepsin

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as

antiviral agents)

IT 85-44-9, Phthalic anhydride 94-09-7, Ethyl 4-aminobenzoate 110-18-9 140-89-6, Potassium ethylxanthate 400-98-6, 4-(Trifluoromethyl)-2-nitroaniline 446-33-3, 3-Fluoro-6-nitrotoluene 455-14-1, 4-(Trifluoromethyl)aniline 583-39-1, 2-Mercaptobenzimidazole 1603-41-4, 2-Amino-5-methylpyridine 1635-61-6, 3-Chloro-6-nitroaniline 1635-84-3, 2,4-Dimethyl-6-nitroaniline 1639-31-2, 3,4,5-Trimethylaniline 1824-81-3, 2-Amino-6-methylpyridine 2127-03-9, 2,2'-Dipyridyl disulfide 3171-45-7, 4,5-Dimethyl-1,2-phenylenediamine 3287-79-4, 2-Mercapto-5,6-dimethylbenzimidazole 5327-33-3, 2-Acetamido-6-methylpyridine 5344-90-1, 2-Aminobenzyl alcohol 7595-31-5 25369-78-2 27231-33-0, 2-Mercapto-4-methylbenzimidazole 27231-36-3 27492-84-8, Methyl 4-amino-2-methoxybenzoate 30525-89-4, Paraformaldehyde 37052-78-1, 2-Mercapto-5-methoxybenzimidazole 39785-37-0, 4-Methoxy-3,5-dimethylaniline 55489-15-1 71675-52-0, 2-(Bromomethyl)-4-chloroaniline hydrobromide 71693-08-8, 2-(Bromomethyl)-5-chloroaniline hydrobromide 74004-74-3 86604-73-1 88301-76-2 88301-77-3 88301-78-4 88301-79-5 88301-81-9, 2-(Chloromethyl)aniline hydrochloride 90562-37-1, N-[2-(Chloromethyl)phenyl]acetamide 92333-53-4 92643-51-1 92807-01-7 106746-59-2, 2-(Chloromethyl)-4-methoxyaniline hydrochloride 106746-62-7 106746-64-9 106746-67-2 106746-71-8 106746-85-4 106746-87-6 106746-89-8 106746-91-2 106746-92-3 106746-99-0 106771-59-9, 2-(Chloromethyl)-N,N-dimethylaniline 174397-86-5 174397-87-6 174397-88-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 4093-29-2P, Methyl 4-acetamido-2-methoxybenzoate 25617-34-9P 27841-33-4P 59338-85-1P, Methyl 4,5-diamino-2-methoxybenzoate 86847-79-2P 104524-65-4P 106746-72-9P 106746-73-0P 106746-74-1P 106746-75-2P 106746-81-0P 106746-82-1P 106746-83-2P 106747-02-8P 106747-03-9P 106747-04-0P 106747-46-0P 106771-57-7P 118267-40-6P 165685-25-6P 174397-89-8P 174397-90-1P 174397-91-2P 174398-21-1P 174398-22-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

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AN 2000:772628 CAPLUS
DN 133:321879
ED Entered STN: 03 Nov 2000
TI Preparation of 5-pyridyl-1,3-azole compounds as antagonists of adenosine A3 receptor, process for producing the same and use thereof
IN Ohkawa, Shigenori; Kanzaki, Naoyuki; Miwatashi, Seiji
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 152 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07D417-04
ICS C07D417-14; A61K031-4439; A61P043-00; A61P029-00; A61P031-12; A61P003-10; A61P001-00; A61P009-00; A61P007-00
CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064894	A1	20001102	WO 2000-JP2575	20000420
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	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1180518	A1	20020220	EP 2000-917375	20000420
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
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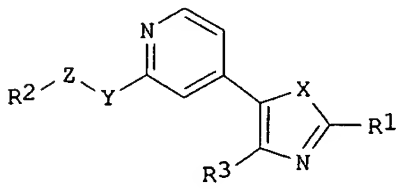
	NZ 515215	A	20030725	NZ 2000-515215	20000420
	AU 765473	B2	20030918	AU 2000-38401	20000420
	JP 2001114779	A2	20010424	JP 2000-126289	20000421
	JP 3333774	B2	20021015		
	JP 2002363179	A2	20021218	JP 2002-164744	20000421
	NO 2001005156	A	20011218	NO 2001-5156	20011022
	ZA 2001008996	A	20030131	ZA 2001-8996	20011031
PRAI	JP 1999-116686	A	19990423		
	JP 1999-224650	A	19990806		
	WO 2000-JP2575	W	20000420		
	JP 2000-126289	A3	20000421		

OS MARPAT 133:321879
GI



I

AB Optionally N-oxidized compds. represented by general formula (I) salts thereof [wherein R1 represents hydrogen, hydrocarbyl, a heterocycle, amino or acyl; R2 represents an arom. group; R3 represents hydrogen, pyridyl or

arom. hydrocarbyl; X represents oxygen or optionally oxidized sulfur; Y represents a bond, oxygen, optionally oxidized sulfur or NR4 (wherein R4 represents hydrogen, hydrocarbyl, or acyl); and Z represents a bond or a divalent chain hydrocarbyl] are prepd. These compds. are usable as preventives or remedies for diseases in assocn. with adenosine A3 receptor because of having excellent adenosine A3 receptor antagonism thereof. Moreover, the compds. I or salts thereof exhibit excellent effects of inhibiting p38 MAP kinase and inhibiting TNF-.alpha. and, therefore, are also usable as preventives or remedies for diseases in assocn. with p38 MAP kinase or TNF-.alpha.. Above diseases include asthma, allergies, brain edema, cerebral vascular disorders, head injuries, inflammation, Addison's disease, autoimmune hemolytic anemia, Crohn's disease, psoriasis, rheumatism, spinal cord injury, multiple sclerosis, Alzheimer's disease, Parkinson's disease, amyotrophic lateral sclerosis, diabetes, arthritis, septemia, ulcerative colitis, chronic pneumonia, silicosis, lung sarcoidosis, pulmonary tuberculosis, cachexia, arteriosclerosis, Creutzfeldt-Jakob disease, virus infection, atopic dermatitis, systemic lupus erythematosus, AIDS encephalopathy, meningitis, angina pectoris, myocardial infarction, ischemic heart failure, hepatitis, transplant, dialysis hypotension, and frequent disseminated intravascular coagulation. Thus, bromination of 2-(2-benzoylamino-4-pyridyl)-1-(4-methoxyphenyl)ethanone with Br in AcOH at room temp. for 1 h followed by cyclocondensation of the bromination product with thiourea in the presence of Et3N in MeCN at 80.degree. for 5 h gave N-[4-[2-amino-4-(4-methoxyphenyl)-1,3-thiazol-5-yl]-2-pyridyl]benzamide (II). II showed IC50 of 0.020 .mu.M against p38 MAP kinase and 0.014 .mu.M for inhibiting the prodn. of TNF-.alpha. in THP-1 cells.

ST pyridylazole prepn antagonist adenosine A3 receptor; pyridylthiazole prepn TNF alpha inhibitor; p38 MAP kinase inhibitor pyridylthiazole

IT Adenosine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(A3; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
Prion diseases
(Creutzfeldt-Jakob; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Intestine, disease
(Crohn's; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Nervous system
(amyotrophic lateral sclerosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease
(angina pectoris; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Dermatitis
(atopic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
(cerebrovascular; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Pneumonia
(chronic; prepn. of pyridylazole compds. as antagonists of adenosine A3

receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Blood coagulation
(disseminated intravascular, frequent; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
(edema; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease
(failure, ischemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Anemia (disease)
(hemolytic, autoimmune; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
(in assocn. with AIDS; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Hypotension
(in assocn. with dialysis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease
(infarction; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Head
Spinal cord
(injury; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Addison's disease
Allergy inhibitors
Alzheimer's disease
Anti-inflammatory agents
Antiarteriosclerotics
Antiarthritics
Antiasthmatics
Antidiabetic agents
Antirheumatic agents
Antiviral agents
Cachexia
Hepatitis
Meningitis
Multiple sclerosis
Parkinson's disease
Psoriasis
Septicemia
Silicosis
Transplant and Transplantation
Tuberculosis
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Tumor necrosis factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lung, disease
(sarcoidosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lupus erythematosus
(systemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Intestine, disease
(ulcerative colitis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-57-4P 303162-71-2P 303162-72-3P 303162-74-5P 303162-75-6P
303162-76-7P 303162-77-8P 303162-78-9P 303162-79-0P 303162-80-3P
303162-85-8P 303162-86-9P 303162-87-0P 303162-88-1P 303162-89-2P
303162-90-5P 303162-91-6P 303162-92-7P 303162-93-8P 303162-94-9P
303162-95-0P 303162-96-1P 303163-15-7P 303163-17-9P 303163-18-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-58-5P 303162-59-6P 303162-60-9P 303162-61-0P 303162-62-1P
303162-64-3P 303162-66-5P 303162-67-6P 303162-68-7P 303162-69-8P
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303163-34-0P 303163-35-1P 303163-36-2P 303163-37-3P 303163-38-4P
303163-39-5P 303163-40-8P 303163-41-9P 303163-42-0P
303163-43-1P 303163-44-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 165245-96-5, p38 MAP kinase
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 62-55-5, Thioacetamide 62-56-6, Thiourea, reactions 64-04-0, 2-Phenylethylamine 74-88-4, Methyl iodide, reactions 75-36-5, Acetyl chloride 75-55-8 98-88-4, Benzoyl chloride 100-07-2, 4-Methoxybenzoyl chloride 100-46-9, Benzylamine, reactions 100-51-6, Benzenemethanol, reactions 100-53-8, Phenylmethanethiol 103-67-3, N-Benzyl-N-methylamine 103-80-0, Phenylacetyl chloride 104-86-9, 4-Chlorobenzylamine 108-98-5, Thiophenol, reactions 109-74-0, Butyronitrile 110-59-8, Valeronitrile 140-75-0, 4-Fluorobenzylamine 499-06-9, 3,5-Dimethylbenzoic acid 589-08-2, N-Methyl-2-phenylethylamine 598-52-7, N-Methylthiourea 631-58-3, Thiopropionamide 645-45-4, 3-Phenylpropionyl chloride 772-70-3, 3-(4-Fluorophenyl)propionyl chloride 873-32-5, 2-Chlorobenzonitrile 1194-02-1, 4-Fluorobenzonitrile 1711-05-3, 3-Methoxybenzoyl chloride 1711-06-4, 3-Methylbenzoyl chloride 2243-83-6, 2-Naphthoyl chloride 2393-23-9, 4-Methoxybenzylamine 2627-86-3, (S)-1-Phenylethylamine 3886-69-9, (R)-1-Phenylethylamine 4152-90-3, 3-Chlorobenzylamine 4926-28-7,

2-Bromo-4-methylpyridine 5071-96-5, 3-Methoxybenzylamine 5271-67-0, 2-Thiophenecarbonyl chloride 6850-57-3, 2-Methoxybenzylamine 15893-42-2, 3-(4-Methoxyphenyl)propionyl chloride 18496-54-3, 4-Phenylbutyryl chloride 20260-53-1, Nicotinoyl chloride hydrochloride 20371-41-9, 5-Phenylvaleryl chloride 21382-98-9, 4-Methylthiobenzonitrile 27757-85-3, 2-Thienylmethylamine 90101-20-5, 2-(tert-Butoxycarbonylamino)-4-methylpyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 461-87-0P, 2-Fluoro-4-methylpyridine 6613-44-1P, 3,5-Dimethylbenzoyl chloride 15717-17-6P, 2-Chlorothiobenzamide 16536-93-9P, Thiobutyramide 16536-94-0P, Thiovaleramide 21384-43-0P 22179-72-2P, 4-Fluorothiobenzamide 53550-91-7P, 4-(Methylthio)thiobenzamide 102336-06-1P 224040-60-2P 224040-71-5P 303162-27-8P 303162-28-9P 303162-29-0P 303162-30-3P 303162-31-4P 303162-32-5P 303162-33-6P 303162-34-7P 303162-35-8P 303162-36-9P 303162-37-0P 303162-38-1P 303162-39-2P 303162-40-5P 303162-41-6P 303162-42-7P 303162-43-8P 303162-44-9P 303162-45-0P 303162-46-1P 303162-47-2P 303162-48-3P 303162-49-4P 303162-50-7P 303162-52-9P 303162-54-1P 303162-55-2P 303162-56-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

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AN 1983:155211 CAPLUS
DN 98:155211
ED Entered STN: 12 May 1984
TI Sulfur-substituted phenoxypyridines having **antiviral** activity
IN Markley, Lowell D.; Tong, Yulan C.; Wood, Steven G.
PA Dow Chemical Co., USA
SO U.S., 22 pp.
CODEN: USXXAM
DT Patent
LA English
IC A61K031-44; C07D021-263
NCL 424263000
CC 1-5 (Pharmacology)
Section cross-reference(s): 27

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4371537	A	19830201	US 1981-292467	19810813
	ZA 8205762	A	19830629	ZA 1982-5762	19820809
	IL 66496	A1	19851129	IL 1982-66496	19820809
	CA 1180017	A1	19841225	CA 1982-409151	19820810
	EP 72529	A1	19830223	EP 1982-107263	19820811
	EP 72529	B1	19860129		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2103619	A1	19830223	GB 1982-23098	19820811
	GB 2103619	B2	19850227		
	AU 8287078	A1	19830512	AU 1982-87078	19820811
	AU 551683	B2	19860508		
	AT 17719	E	19860215	AT 1982-107263	19820811
	NO 8202751	A	19830214	NO 1982-2751	19820812
	NO 159851	B	19881107		
	NO 159851	C	19890215		
	DK 8203628	A	19830214	DK 1982-3628	19820812
	DK 157297	B	19891204		
	DK 157297	C	19900507		
	JP 58041868	A2	19830311	JP 1982-139277	19820812
	JP 04014107	B4	19920311		
	ES 514940	A1	19831016	ES 1982-514940	19820812
	ES 523661	A1	19850316	ES 1983-523661	19830628
	ES 523660	A1	19850401	ES 1983-523660	19830628
PRAI	US 1981-292467		19810813		
	EP 1982-107263		19820811		

OS CASREACT 98:155211
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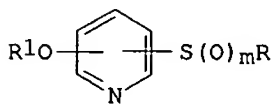

I

AB The title compds. I [R = C1-7 alkyl, C5 or C6 cycloalkyl, Ar(CH2)q (Ar = C6-10 aryl, q = 0-3), R1 = Ph or substituted Ph; m = 0, 1, or 2] preferably administered as pharmaceutical compns. (no data given) were prepd. by several methods and evaluated as **antiviral** agents. Thus, 2-(3,4-dichlorophenoxy)-5-(methylsulfonyl)pyridine [85331-30-2] prepd. by the reaction of 3,4-dichlorophenol [95-77-2] in DMSO in presence of Na tert-butoxide with 2,5-bis(methylsulfonyl)pyridine showed a

broad spectrum **antiviral** activity at low conc. (25 .mu.g/mL).

ST phenoxythiopyridine prepn **antiviral**; virucide
phenoxythiopyridine; pyridine phenoxythio prepn **antiviral**

IT Virucides and Virustats
(phenoxythiopyridines)

IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**
85331-31-3P 85331-32-4P 85331-38-0P 85331-39-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation of)

IT 85331-36-8P 85331-37-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

IT 58819-71-9P 71506-85-9P 85330-62-7P 85330-65-0P 85330-68-3P
85330-69-4P 85330-71-8P 85330-74-1P **85330-77-4P**
85330-81-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

IT 85331-34-6P 85331-35-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with dichlorophenol)

IT 85330-72-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with hydroxyacetophenone)

IT **85330-78-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with hydroxybenzophenone)

IT 25935-30-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with sodium methanethiolate)

IT 85330-63-8P 85330-64-9P 85330-66-1P 85330-75-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with substituted phenols)

IT 25935-29-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)

IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P
85330-89-8P 85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P
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85331-19-7P 85331-20-0P 85331-21-1P 85331-22-2P 85331-23-3P
85331-24-4P 85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P
85331-29-9P 85331-30-2P 85345-64-8P 85368-98-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and virucidal activity)

IT 62916-42-1P 85330-79-6P 85330-80-9P 85330-82-1P 85330-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 75-33-2
RL: BIOL (Biological study)
(reaction of with Me dichloropyridinecarboxylate)

IT 100-53-8 108-98-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Me dichloropyridinecarboxylate)
IT 95-95-4 533-31-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(ethylsulfonyl)pyridine)
IT 98-54-4 99-93-4 101-53-1 106-41-2 106-48-9 461-84-7 591-20-8
767-00-0 831-82-3 873-62-1 1073-72-9 1137-42-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(methylsulfonyl)pyridine)
IT 95-77-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloronitropyridine)
IT 140-89-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diazotized pyridine derivs.)
IT 4548-45-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichlorophenol)
IT 1569-69-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichloropyridinecarboxylic acid)
IT 75-08-1 111-31-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichlorpyridinecarboxylic acid)
IT 1532-24-7 1702-17-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with mercaptans)
IT 26452-80-2 85331-33-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methanethiol)
IT 74-93-1, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pyridinecarboxylates)

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AN 1999:705001 CAPLUS
DN 131:322530
ED Entered STN: 04 Nov 1999
TI Substituted tetronic acids useful for treating **HIV** and other retroviruses
IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin, James M.; Smith, Clark W.; Tommasi, Ruben A.; Aristoff, Paul A.; Skulnick, Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.
PA USA
SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 238,820, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-34
ICS A61K031-335; A61K031-415; A61K031-505
NCL 514473000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5977169	A	19991102	US 1997-604937	19970728
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	WO 9507901	A1	19950323	WO 1994-US9533	19940907

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

PRAI US 1993-123029 19930917
US 1994-238820 19940506
WO 1994-US9533 19940907
OS MARPAT 131:322530
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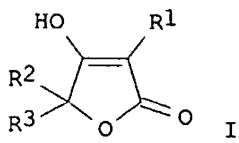

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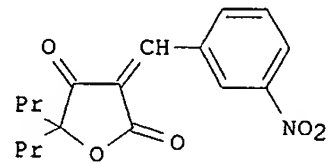
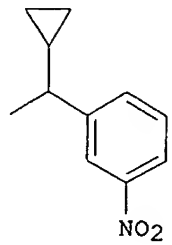
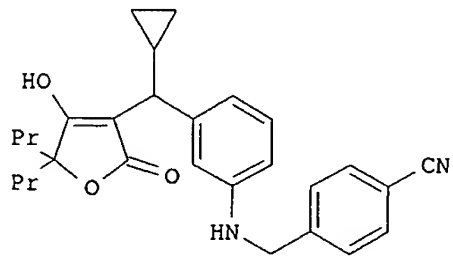


II

Q1=





III

AB The invention comprises novel substituted tetronic acid derivs. (I) and tautomers [wherein R1-R3 = wide variety of specified C-contg. substituents] that are inhibitors of **HIV** protease. I retard replication of any **retrovirus** contg. aspartyl protease and are

useful for treatment of AIDS or AIDS-related diseases. Approx. 250 compds. are claimed, and phys. and biol. data for approx. 120 compds. are provided. For example, condensation of I [R1 = H, R2 = R3 = Pr] with 3-nitrobenzaldehyde gave >100% crude nitrobenzylidene deriv. II, which reacted with cyclopropylmagnesium bromide and CuBr.SMe2 in THF to give 62% I [R1 = Q1, R2 = R3 = Pr]. Hydrogenation of the nitro group (97%) and sulfonamidation of the resultant amino group with 4-cyanobenzenesulfonyl chloride (53%) gave title furandione III, a preferred compd. Several compds. including III are said to have inhibited replication of **HIV**-1IIIB in human cell lines. **HIV**-1 protease inhibitory data are provided, and over 100% inhibition was reported for many test compds. at doses as low as 3.3 .mu.M.

ST tetronic acid prepn antiviral **retrovirus** replication inhibitor; furandione prepn antiviral **retrovirus** replication inhibitor; **HIV** protease inhibitor AIDS treatment tetronic acid prepn

IT Human immunodeficiency virus
Human immunodeficiency virus 1
(inhibition; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT Anti-AIDS agents
Antiviral agents
(prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT AIDS (disease)
(treatment; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 144114-21-6, Retropepsin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 1138-44-9P 10424-93-8P 72036-34-1P 85520-35-0P 161720-04-3P
164346-90-1P 164346-91-2P 164346-92-3P 164346-93-4P 164346-94-5P
164346-95-6P 164346-96-7P 164346-98-9P 164346-99-0P 164347-01-7P
164347-02-8P 164347-03-9P 164347-07-3P 164347-10-8P 248608-58-4P
248608-59-5P 248608-60-8P 248608-61-9P 248608-62-0P 248608-63-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 99-61-6, 3-Nitrobenzaldehyde 100-39-0, Benzyl bromide 103-63-9, (2-Bromoethyl)benzene 104-53-0, Hydrocinnamaldehyde 106-94-5 108-94-1, Cyclohexanone, reactions 109-72-8, n-Butyl lithium, reactions 120-92-3, Cyclopentanone 502-49-8, Cyclooctanone 623-47-2, Ethyl propiolate 637-59-2, 1-Bromo-3-phenylpropane 946-33-8, 2-Benzylcyclohexanone 1007-03-0, .alpha.-Cyclopropylbenzyl alcohol 1067-74-9, Methyl diethylphosphonoacetate 2550-26-7, Benzyl acetone 2637-37-8, 2-Quinolinethiol 4423-94-3, 2-Ethylcyclohexanone 4971-56-6, Tetronic acid 14371-10-9 23719-80-4, Cyclopropylmagnesium bromide 29976-53-2, 1-Carbethoxy-4-piperidone 49584-26-1, 4-Cyanobenzenesulfonyl chloride 118753-70-1 135005-10-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 164344-46-1P 164344-47-2P 164344-48-3P 164344-49-4P 164344-50-7P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 248608-46-0P 248608-48-2P 248608-49-3P 248608-50-6P 248608-51-7P
248608-52-8P 248608-53-9P 248608-54-0P 248608-56-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(3) Anon; 1963
(4) Anon; 1965
(5) Anon; 1977 CAPLUS
(6) Anon; 1979 CAPLUS
(7) Anon; 1979 CAPLUS

(8) Anon; 1979 CAPLUS
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(10) Anon; 1983 CAPLUS
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(16) Anon; 1993 CAPLUS
(17) Anon; JP 05-043568 1993 CAPLUS
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(19) Anon; WO 9304055 1993 CAPLUS
(20) Anon; WO 9411361 1994 CAPLUS
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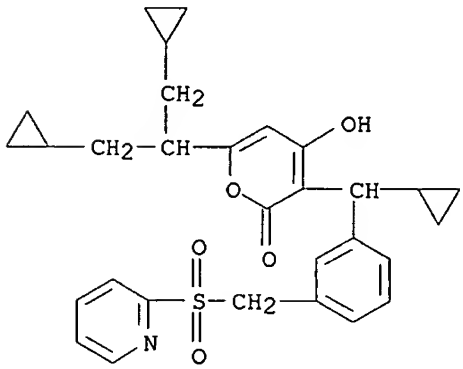
AN 1997:165733 CAPLUS
DN 126:258470
ED Entered STN: 12 Mar 1997
TI Synthesis and pharmacological evaluation of sulfone substituted **HIV** protease inhibitors
AU Schwartz, Theresa M.; Bundy, Gordon L.; Strohbach, Joseph W.; Thairrivongs, Suvit; Johnson, Paul D.; Skulnick, Harvey I.; Tomich, Paul K.; Lynn, Janet C.; Chong, Kong Teck; Hinshaw, Roger R.; Raub, Thomas J.; Padbury, Guy E.; Loth, Lisa N.
CS Res. Labs., Pharmacia Upjohn, Inc., Kalamazoo, MI, 49001-0199, USA
SO Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 399-402
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier
DT Journal
LA English
CC 1-3 (Pharmacology)
AB The sulfonamide substituted pyranones (1) have recently been shown to be potent **HIV** protease inhibitors. We prepard a series of sulfone substituted analogs and compared and their biol. activities to those of the corresponding sulfonamide analogs. It was detd. that although these compds. maintained activity as enzyme inhibitors, they showed somewhat diminished antiviral activity event though they may possess increased membrane permeability.
ST sulfonamide pyranone prepn **HIV** protease inhibitor
IT Structure-activity relationship
(antiviral; sulfonamide substituted pyranones as **HIV** protease inhibitors)
IT Structure-activity relationship
(aspartic proteinase-inhibiting; sulfonamide substituted pyranones as **HIV** protease inhibitors)
IT Anti-AIDS agents
Antiviral agents
Human immunodeficiency virus 1
(sulfonamide substituted pyranones as **HIV** protease inhibitors)
IT 174483-90-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antiviral and **HIV**-1 protease inhibiting activity of)
IT 166335-18-8P 166335-24-6P 166335-32-6P 166335-74-6P 166335-80-4P
174483-25-1P 174483-26-2P 174483-27-3P 174483-28-4P 174483-29-5P
174483-30-8P 174483-56-8P 174483-62-6P 174483-63-7P 174483-94-4P
188839-13-6P 188839-14-7P 188839-15-8P **188839-16-9P**
188839-17-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antiviral and **HIV**-1 protease inhibiting activity of)
IT 162174-73-4P 174484-94-7P 188839-19-2P 188839-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of)
IT 675-10-5 7051-34-5, Bromomethyl cyclopropane 100058-82-0 174484-93-6
188839-18-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of)
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Chong, K; Antimicrob Agents Chemother 1994, V38, P288 CAPLUS
(2) Conradi, R; Pharm Res 1991, V8, P1453 CAPLUS
(3) Nogami, H; Chem Pharm Bull 1968, V16, P580 CAPLUS

(4) Raub, T; Unpublished result
(5) Romines, K; Curr Med Chem 1995, V2, P825 CAPLUS
(6) Romines, K; J Med Chem 1995, V38, P4463 CAPLUS
(7) Sawada, G; Pharm Res 1994, V11, P665 CAPLUS
(8) Skulnick, H; J Med Chem 1995, V38, P4968 CAPLUS
(9) Skulnick, H; J Med Chem, in press
(10) Thaisrivongs, S; J Med Chem 1994, V37, P3200 CAPLUS
(11) Thaisrivongs, S; J Med Chem 1996, V39, P2400 CAPLUS

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN **188839-16-9** REGISTRY
CN 2H-Pyran-2-one, 6-[2-cyclopropyl-1-(cyclopropylmethyl)ethyl]-3-[cyclopropyl[3-[(2-pyridinylsulfonyl)methyl]phenyl]methyl]-4-hydroxy-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H33 N O5 S
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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AN 2002:974259 CAPLUS
DN 138:33310
ED Entered STN: 26 Dec 2002
TI Antiretroviral compounds and compositions
IN Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweyko, Arthur M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise Jones Howard L.; Harrison, William A.
PA Uniroyal Chemical Company, Inc., USA
SO U.S., 19 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-47
ICS C07D215-16; C07D211-72; C07D211-84
NCL 546157000; 546290000; 546294000; 514312000; 514345000; 514347000
CC 1-5 (Pharmacology)
Section cross-reference(s): 27
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498254	B1	20021224	US 2001-21202	20011029
	WO 2003037866	A1	20030508	WO 2002-US29573	20020917
	W: AU, BR, CA, CN, JP, MX				
PRAI	US 2001-21202	A	20011029		

AB Certain pyridine and quinoline derivs. which inhibit replication of the retroviruses HIV-1, HIV-2 and human cytomegalovirus (HCMV) are provided. Pharmaceutical compns. useful in methods of treating or inhibiting certain retrovirus infections are described.
ST antiretroviral compd pyridine quinoline deriv
IT Anti-AIDS agents
Antiviral agents
Human
Human herpesvirus 5
Human immunodeficiency virus 1
Human immunodeficiency virus 2
(antiretroviral compds. and compns. using pyridine and quinoline derivs.)
IT Drug delivery systems
(carriers; antiretroviral compds. and compns. using pyridine and quinoline derivs.)
IT 478620-19-8P 478620-24-5P 478620-25-6P 478620-28-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antiretroviral compds. and compns. using pyridine and quinoline derivs.)
IT 69212-31-3P, 2-Benzylthio-3-nitropyridine 478619-45-3P 478619-49-7P
478619-53-3P 478619-57-7P 478619-61-3P 478619-65-7P 478619-68-0P
478619-72-6P 478619-78-2P 478619-82-8P 478619-86-2P 478619-90-8P
478619-94-2P 478619-98-6P 478620-02-9P 478620-06-3P 478620-08-5P
478620-11-0P 478620-12-1P 478620-14-3P 478620-16-5P 478620-18-7P
478620-20-1P 478620-21-2P 478620-23-4P 478620-26-7P 478620-27-8P
478620-29-0P 478620-30-3P 478620-31-4P 478620-32-5P 478620-33-6P
478620-34-7P 478620-35-8P 478620-36-9P 478620-37-0P 478620-38-1P
478620-39-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiretroviral compds. and compns. using pyridine and quinoline derivs.)
IT 51-79-6, Urethane 86-81-7, 3,4,5-Trimethoxybenzaldehyde 100-44-7, Benzyl chloride, reactions 100-52-7, Benzaldehyde, reactions 100-53-8,

Benzylmercaptan 123-11-5, 4-Methoxybenzaldehyde, reactions 607-66-9, 2-Hydroxy-4-methylquinoline 824-45-3, 2,5-Dimethylbenzyl chloride 2014-83-7, 2,6-Dichlorobenzyl chloride 2044-27-1, 1-Methyl-2(1H)-pyridinethione 2587-00-0, 2,6-Dichloropyridine-N-oxide 2637-34-5, 2-Mercaptopyridine 3811-73-2 5470-18-8, 2-Chloro-3-nitropyridine 6258-60-2, 4-Methoxybenzylmercaptan 20871-93-6 22182-98-5 52694-50-5, 3-Chloromethyl-1-methylpiperidine 53976-62-8 53976-65-1 60263-88-9 82959-54-4 84504-48-3 91668-83-6, 2-Chloro-3-methylpyridine-N-oxide 338778-95-3 478619-47-5 478619-51-1 **478619-55-5** 478619-59-9 478619-63-5 478619-70-4 478619-76-0 478619-80-6 478619-84-0 478619-88-4 478619-92-0 478619-96-4 478620-00-7 478620-05-2 478620-07-4 478620-09-6 478620-10-9 478620-13-2 478620-15-4 478620-17-6 478620-22-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(antiretroviral compds. and compns. using pyridine and quinoline derivs.)

IT 4437-65-4P 81167-65-9P 81167-66-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(antiretroviral compds. and compns. using pyridine and quinoline derivs.)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Brouwer; US 5696151 A 1997 CAPLUS
(2) Harrison; US 5268389 A 1993 CAPLUS
(3) Moormann; US 5945425 A 1999 CAPLUS

=>

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                   present
 NEWS  4  DEC 08   INPADOC: Legal Status data reloaded
 NEWS  5  SEP 29   DISSABS now available on STN
 NEWS  6  OCT 10   PCTFULL: Two new display fields added
 NEWS  7  OCT 21   BIOSIS file reloaded and enhanced
 NEWS  8  OCT 28   BIOSIS file segment of TOXCENTER reloaded and enhanced
 NEWS  9  NOV 24   MSDS-CCOHS file reloaded
 NEWS 10  DEC 08   CABA reloaded with left truncation
 NEWS 11  DEC 08   IMS file names changed
 NEWS 12  DEC 09   Experimental property data collected by CAS now available
                   in REGISTRY
 NEWS 13  DEC 09   STN Entry Date available for display in REGISTRY and CA/CAplus
 NEWS 14  DEC 17   DGENE: Two new display fields added
 NEWS 15  DEC 18   BIOTECHNO no longer updated
 NEWS 16  DEC 19   CROPU no longer updated; subscriber discount no longer
                   available
 NEWS 17  DEC 22   Additional INPI reactions and pre-1907 documents added to CAS
                   databases
 NEWS 18  DEC 22   IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
 NEWS 19  DEC 22   ABI-INFORM now available on STN

 NEWS EXPRESS  DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
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=> file reg
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COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                          ENTRY    SESSION
FULL ESTIMATED COST                                        0.21       0.21

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STRUCTURE FILE UPDATES:   20 JAN 2004  HIGHEST RN 639777-15-4
DICTIONARY FILE UPDATES:  20 JAN 2004  HIGHEST RN 639777-15-4

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http://www.cas.org/ONLINE/DBSS/registryss.html

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Uploading 021453.str

L1      STRUCTURE UPLOADED

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L1 HAS NO ANSWERS
L1                STR
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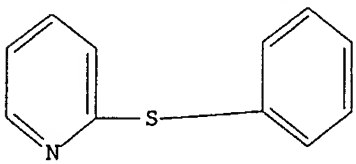


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Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SCREEN SEARCH COMPLETED -     25 TO ITERATE

100.0% PROCESSED      25 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          200 TO      800
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA EXA SAM L1

=> s l1 fam sam
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SAMPLE SEARCH INITIATED 09:21:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 672 TO 1568
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA FAM SAM L1

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SAMPLE SCREEN SEARCH COMPLETED - 552 TO ITERATE

100.0% PROCESSED 552 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

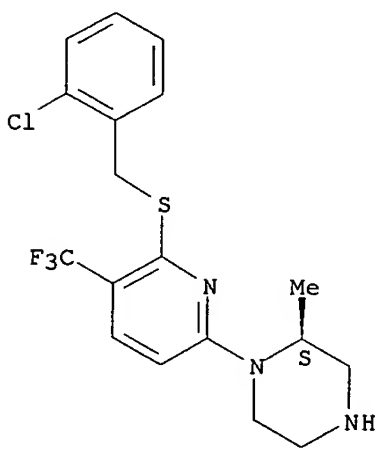
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9631 TO 12449
PROJECTED ANSWERS: 3098 TO 4782

L4 50 SEA SSS SAM L1

=> d l4 1-50

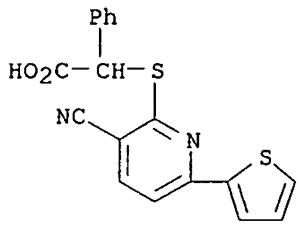
L4 ANSWER 1 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 625844-46-4 REGISTRY
CN Piperazine, 1-[6-[[(2-chlorophenyl)methyl]thio]-5-(trifluoromethyl)-2-pyridinyl]-2-methyl-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H19 Cl F3 N3 S
CI COM
SR CA

Absolute stereochemistry.



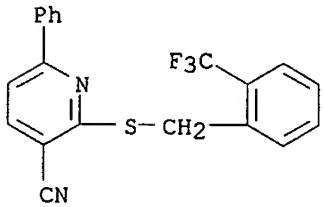
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 2 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 625375-04-4 REGISTRY
CN Benzeneacetic acid, .alpha.-[[3-cyano-6-(2-thienyl)-2-pyridinyl]thio]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H12 N2 O2 S2
SR Chemical Library
LC STN Files: CHEMCATS



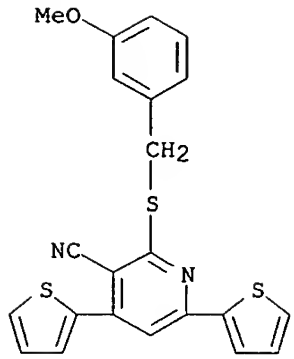
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 3 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 625371-98-4 REGISTRY
CN 3-Pyridinecarbonitrile, 6-phenyl-2-[[[2-(trifluoromethyl)phenyl]methyl]thi
o]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H13 F3 N2 S
SR Chemical Library
LC STN Files: CHEMCATS



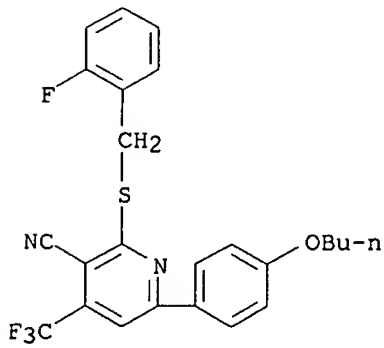
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 4 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 625371-35-9 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(3-methoxyphenyl)methyl]thio]-4,6-di-2-thienyl-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H16 N2 O S3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 5 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 608494-96-8 REGISTRY
CN 3-Pyridinecarbonitrile, 6-(4-butoxyphenyl)-2-[[(2-fluorophenyl)methyl]thio]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H20 F4 N2 O S
SR Chemical Library
LC STN Files: CHEMCATS



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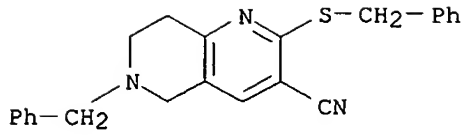
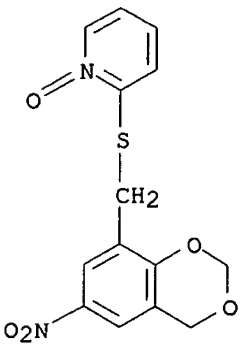
L4 ANSWER 6 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 607698-12-4 REGISTRY
CN 1,6-Naphthyridine-3-carbonitrile, 5,6,7,8-tetrahydro-6-(phenylmethyl)-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H21 N3 S
SR Chemical Library
LC STN Files: CHEMCATS



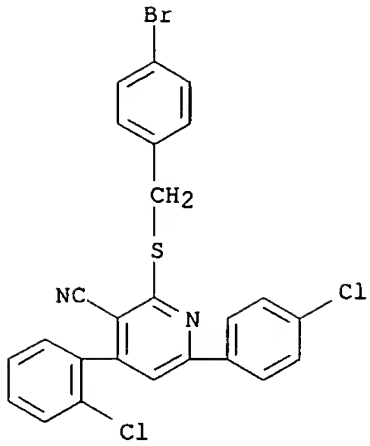
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 7 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 556022-40-3 REGISTRY
CN Pyridine, 2-[[(6-nitro-4H-1,3-benzodioxin-8-yl)methyl]thio]-, 1-oxide (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H12 N2 O5 S
SR Chemical Library
LC STN Files: CHEMCATS



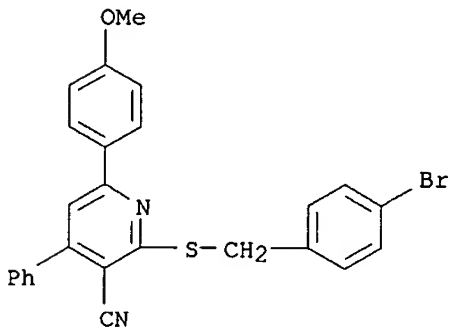
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 8 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 553658-94-9 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(4-bromophenyl)methyl]thio]-4-(2-chlorophenyl)-6-(4-chlorophenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C25 H15 Br Cl2 N2 S
SR Chemical Library
LC STN Files: CHEMCATS



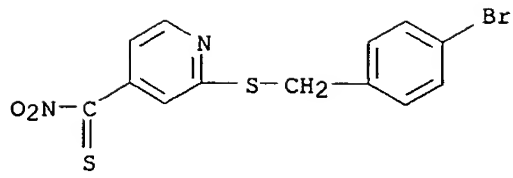
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 9 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 553658-93-8 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(4-bromophenyl)methyl]thio]-6-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H19 Br N2 O S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 10 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 537656-95-4 REGISTRY
CN 4-Pyridinecarbothioaldehyde, 2-[[(4-bromophenyl)methyl]thio]-.alpha.-nitro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H9 Br N2 O2 S2
SR CA
LC STN Files: CA, CAPLUS



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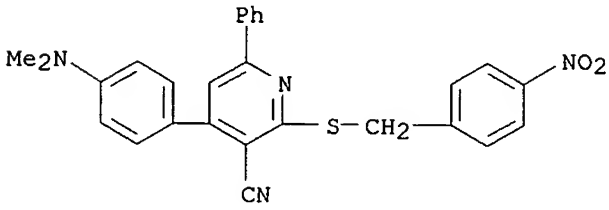
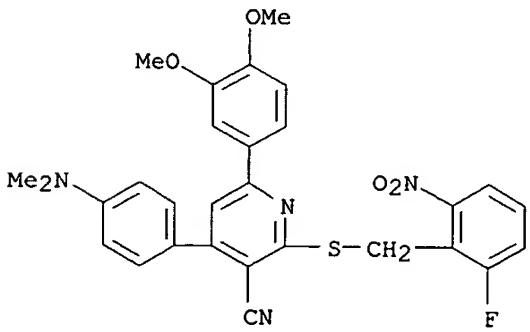
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 11 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 514853-30-6 REGISTRY
CN 3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-2-[[(4-nitrophenyl)methyl]thio]-6-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H22 N4 O2 S
SR Chemical Library
LC STN Files: CHEMCATS



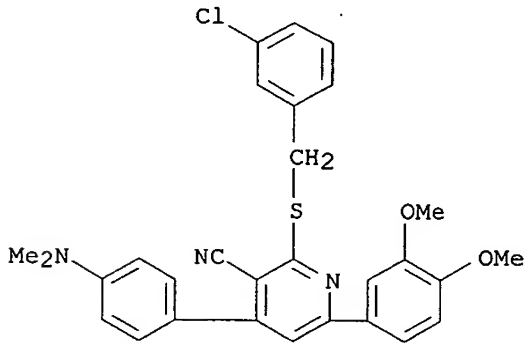
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 12 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 514852-33-6 REGISTRY
CN 3-Pyridinecarbonitrile, 6-(3,4-dimethoxyphenyl)-4-[4-(dimethylamino)phenyl]-2-[[(2-fluoro-6-nitrophenyl)methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H25 F N4 O4 S
SR Chemical Library
LC STN Files: CHEMCATS



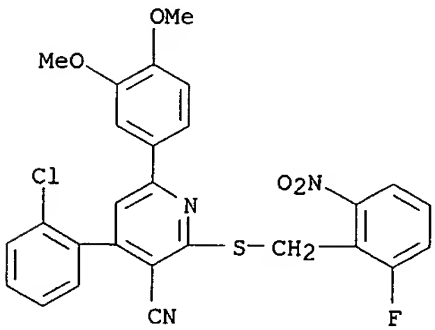
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 13 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 514851-98-0 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(3-chlorophenyl)methyl]thio]-6-(3,4-dimethoxyphenyl)-4-[4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H26 Cl N3 O2 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

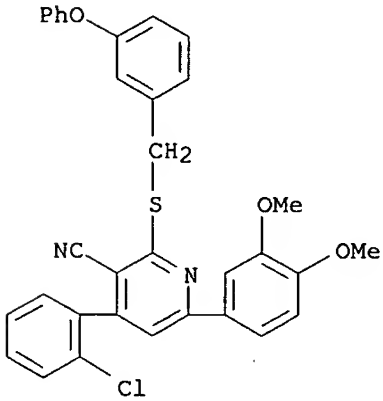
L4 ANSWER 14 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 514851-49-1 REGISTRY
CN 3-Pyridinecarbonitrile, 4-(2-chlorophenyl)-6-(3,4-dimethoxyphenyl)-2-[[(2-fluoro-6-nitrophenyl)methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H19 Cl F N3 O4 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

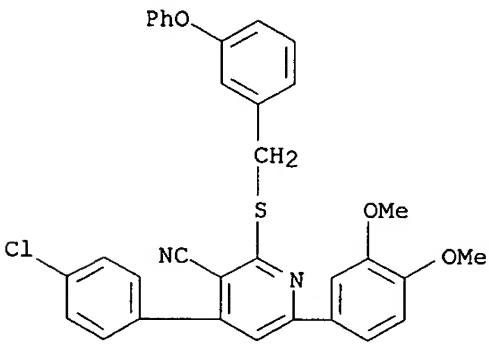
L4 ANSWER 15 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 514851-39-9 REGISTRY

CN 3-Pyridinecarbonitrile, 4-(2-chlorophenyl)-6-(3,4-dimethoxyphenyl)-2-[[(3-phenoxyphenyl)methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H25 Cl N2 O3 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

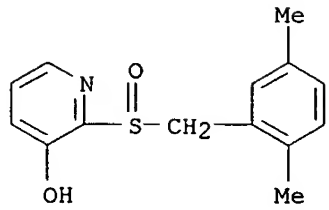
L4 ANSWER 16 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 514850-93-2 REGISTRY
CN 3-Pyridinecarbonitrile, 4-(4-chlorophenyl)-6-(3,4-dimethoxyphenyl)-2-[[(3-phenoxyphenyl)methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H25 Cl N2 O3 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 17 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 500163-27-9 REGISTRY
CN 3-Pyridinol, 2-[[(2,5-dimethylphenyl)methyl]sulfinyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H15 N O2 S

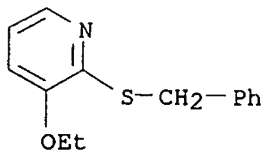
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 18 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 500163-13-3 REGISTRY
CN Pyridine, 3-ethoxy-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H15 N O S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

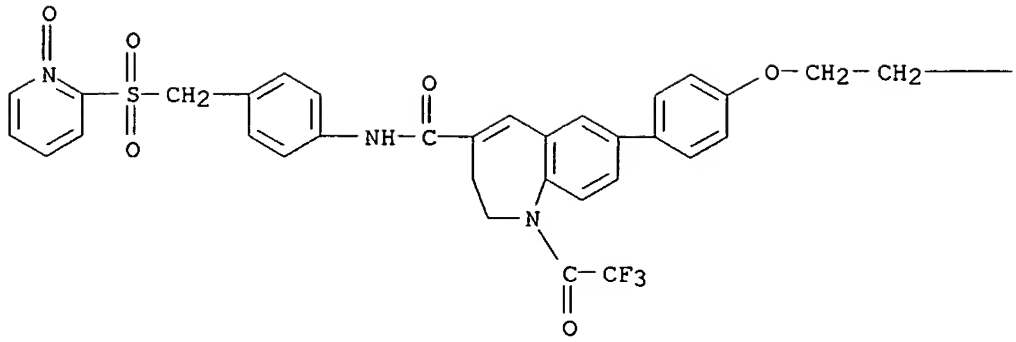


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 19 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 497851-00-0 REGISTRY
CN 1H-1-Benzazepine-4-carboxamide, 7-[4-(2-butoxyethoxy)phenyl]-2,3-dihydro-N-[4-[[(1-oxido-2-pyridinyl)sulfonyl]methyl]phenyl]-1-(trifluoroacetyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C37 H36 F3 N3 O7 S
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

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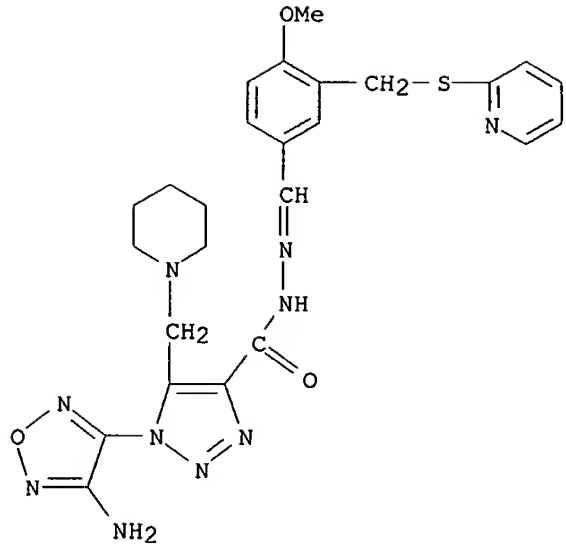
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

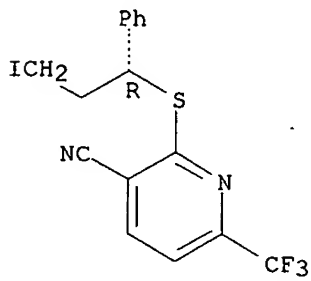
L4 ANSWER 20 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 497246-37-4 REGISTRY
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(4-amino-1,2,5-oxadiazol-3-yl)-5-(1-piperidinylmethyl)-, [[4-methoxy-3-[(2-pyridinylthio)methyl]phenyl]methylene]hydrazide (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C25 H28 N10 O3 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 21 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 496871-24-0 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(1R)-3-iodo-1-phenylpropyl]thio]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H12 F3 I N2 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



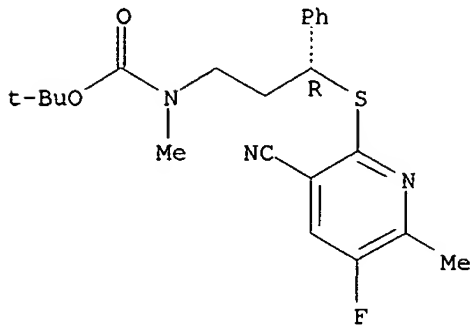
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 22 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 496871-22-8 REGISTRY
CN Carbamic acid, [(3R)-3-[(3-cyano-5-fluoro-6-methyl-2-pyridinyl)thio]-3-phenylpropyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H26 F N3 O2 S
SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

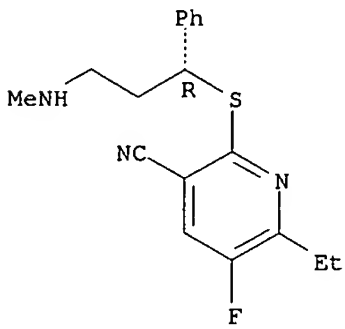


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 23 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 496870-29-2 REGISTRY
CN 3-Pyridinecarbonitrile, 6-ethyl-5-fluoro-2-[[(1R)-3-(methylamino)-1-phenylpropyl]thio]-, dihydrochloride (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H20 F N3 S . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (496870-54-3)

Absolute stereochemistry.

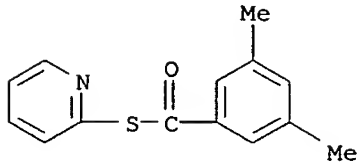


●2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 24 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 496067-45-9 REGISTRY
CN Benzenecarbothioic acid, 3,5-dimethyl-, S-2-pyridinyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD

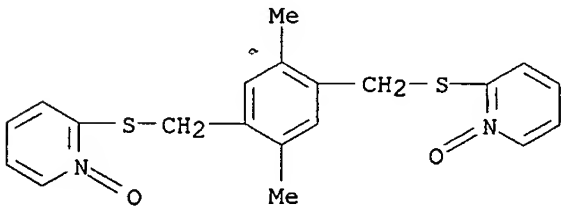
MF C14 H13 N O S
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

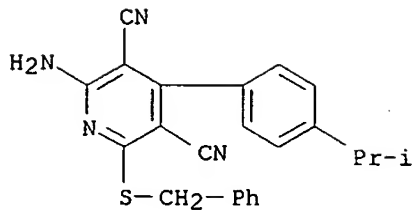
L4 ANSWER 25 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 478619-55-5 REGISTRY
CN Pyridine, 2,2'-[(2,5-dimethyl-1,4-phenylene)bis(methylenethio)]bis-, 1,1'-dioxide (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H20 N2 O2 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

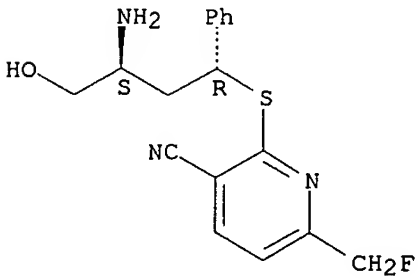
L4 ANSWER 26 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 476319-21-8 REGISTRY
CN 3,5-Pyridinedicarbonitrile, 2-amino-4-[4-(1-methylethyl)phenyl]-6-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H20 N4 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 27 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 474823-65-9 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-6-(fluoromethyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-[((1R,3S)-3-Amino-4-hydroxy-1-phenylbutyl)thio]-6-(fluoromethyl)-3-pyridinecarbonitrile
FS STEREOSEARCH
MF C17 H18 F N3 O S
CI COM
SR CA
LC STN Files: CA, CAPLUS

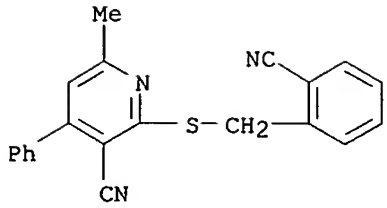
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

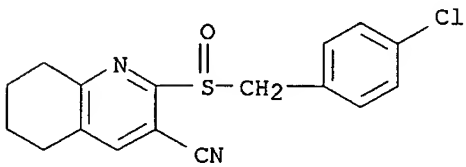
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 28 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 459182-40-2 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(2-cyanophenyl)methyl]thio]-6-methyl-4-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H15 N3 S
SR Chemical Library
LC STN Files: CHEMCATS



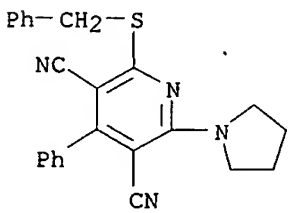
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 29 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 459154-94-0 REGISTRY
CN 3-Quinolinecarbonitrile, 2-[[(4-chlorophenyl)methyl]sulfinyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H15 Cl N2 O S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

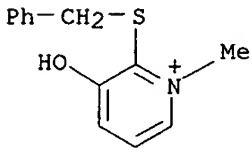
L4 ANSWER 30 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 455877-30-2 REGISTRY
CN 3,5-Pyridinedicarbonitrile, 4-phenyl-2-[(phenylmethyl)thio]-6-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H20 N4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

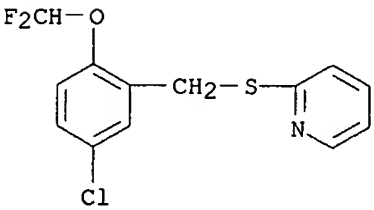
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 31 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 454421-81-9 REGISTRY
CN Pyridinium, 3-hydroxy-1-methyl-2-[(phenylmethyl)thio]-, bromide (9CI) (CA INDEX NAME)
MF C13 H14 N O S . Br
SR Chemical Library
LC STN Files: CHEMCATS



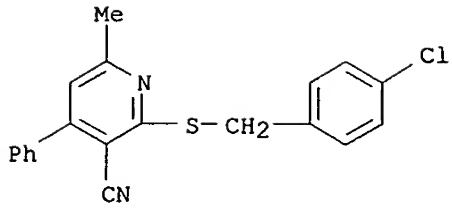
● Br^-

L4 ANSWER 32 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 452299-62-6 REGISTRY
CN Pyridine, 2-[[[5-chloro-2-(difluoromethoxy)phenyl]methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H10 Cl F2 N O S
SR Chemical Library
LC STN Files: CHEMCATS



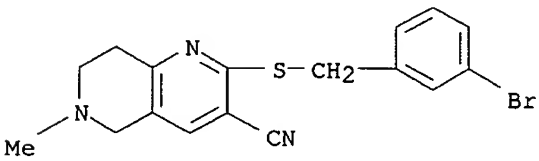
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 33 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 449748-57-6 REGISTRY
CN 3-Pyridinecarbonitrile, 2-[[(4-chlorophenyl)methyl]thio]-6-methyl-4-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H15 Cl N2 S
SR Chemical Library
LC STN Files: CHEMCATS



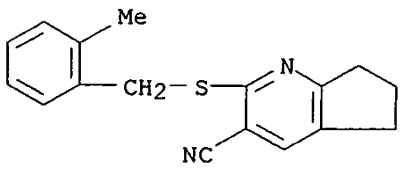
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 34 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 445383-68-6 REGISTRY
CN 1,6-Naphthyridine-3-carbonitrile, 2-[[(3-bromophenyl)methyl]thio]-5,6,7,8-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 Br N3 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

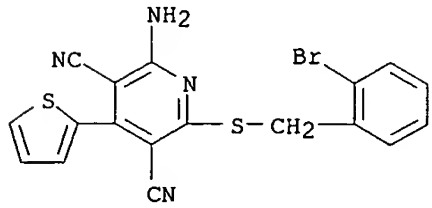
L4 ANSWER 35 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 445383-65-3 REGISTRY
CN 5H-Cyclopenta[b]pyridine-3-carbonitrile, 6,7-dihydro-2-[[(2-methylphenyl)methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H16 N2 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

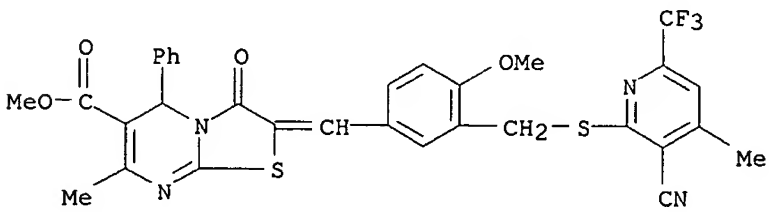
L4 ANSWER 36 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 445381-37-3 REGISTRY
CN 3,5-Pyridinedicarbonitrile, 2-amino-6-[[(2-bromophenyl)methyl]thio]-4-(2-thienyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD
MF C18 H11 Br N4 S2
SR Chemical Library
LC STN Files: CHEMCATS



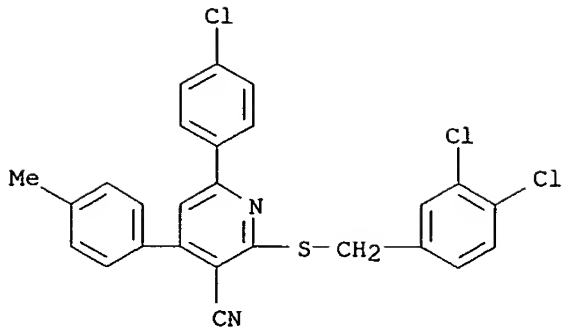
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 37 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 445244-89-3 REGISTRY
CN 5H-Thiazolo[3,2-a]pyrimidine-6-carboxylic acid, 2-[[3-[[[3-cyano-4-methyl-6-(trifluoromethyl)-2-pyridinyl]thio]methyl]-4-methoxyphenyl]methylene]-2,3-dihydro-7-methyl-3-oxo-5-phenyl-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H25 F3 N4 O4 S2
SR Chemical Library
LC STN Files: CHEMCATS



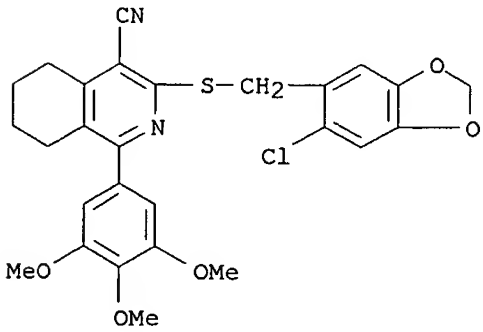
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 38 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 444156-75-6 REGISTRY
CN 3-Pyridinecarbonitrile, 6-(4-chlorophenyl)-2-[[(3,4-dichlorophenyl)methyl]thio]-4-(4-methylphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H17 Cl3 N2 S
SR Chemical Library
LC STN Files: CHEMCATS



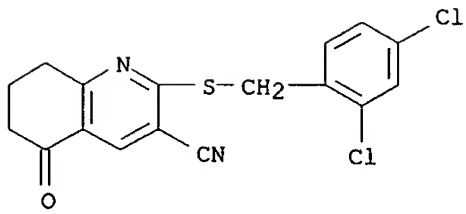
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 39 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 444151-34-2 REGISTRY
CN 4-Isoquinolinecarbonitrile, 3-[[(6-chloro-1,3-benzodioxol-5-yl)methyl]thio]-5,6,7,8-tetrahydro-1-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H25 Cl N2 O5 S
SR Chemical Library
LC STN Files: CHEMCATS



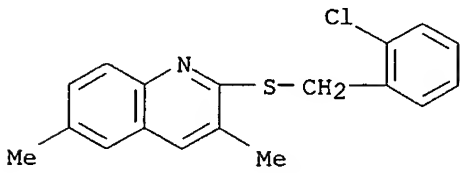
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 40 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 444079-11-2 REGISTRY
CN 3-Quinolinecarbonitrile, 2-[[(2,4-dichlorophenyl)methyl]thio]-5,6,7,8-tetrahydro-5-oxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H12 Cl2 N2 O S
SR Chemical Library
LC STN Files: CHEMCATS



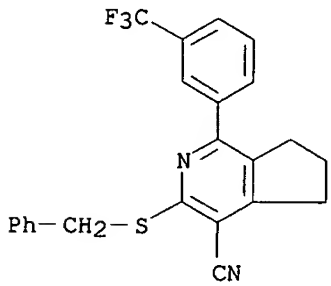
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 41 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 443745-43-5 REGISTRY
CN Quinoline, 2-[[(2-chlorophenyl)methyl]thio]-3,6-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H16 Cl N S
SR Chemical Library
LC STN Files: CHEMCATS



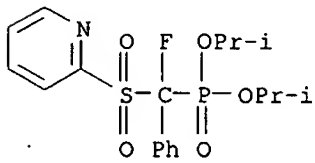
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 42 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 439108-57-3 REGISTRY
CN 5H-Cyclopenta[c]pyridine-4-carbonitrile, 6,7-dihydro-3-[(phenylmethyl)thio]-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H17 F3 N2 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

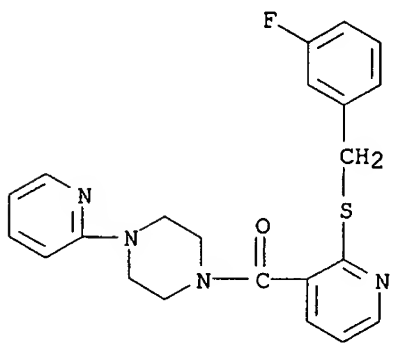
L4 ANSWER 43 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 428867-21-4 REGISTRY
CN Phosphonic acid, [fluorophenyl(2-pyridinylsulfonyl)methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Diisopropyl [Fluoro(phenyl)(pyridin-2-ylsulfonyl)methyl]phosphonate
FS 3D CONCORD
MF C18 H23 F N O5 P S
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

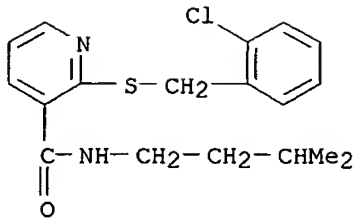
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 44 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 423146-99-0 REGISTRY
CN Piperazine, 1-[[2-[[(3-fluorophenyl)methyl]thio]-3-pyridinyl]carbonyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H21 F N4 O S
SR Chemical Library
LC STN Files: CHEMCATS



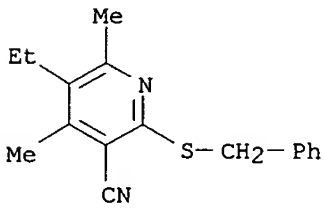
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 45 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 423146-88-7 REGISTRY
CN 3-Pyridinecarboxamide, 2-[[(2-chlorophenyl)methyl]thio]-N-(3-methylbutyl)-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 Cl N2 O S
SR Chemical Library
LC STN Files: CHEMCATS



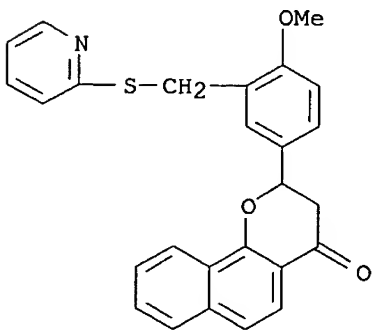
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

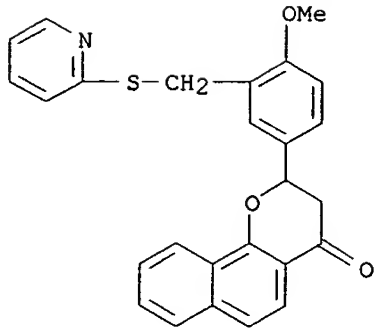
L4 ANSWER 46 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 413606-89-0 REGISTRY
CN 3-Pyridinecarbonitrile, 5-ethyl-4,6-dimethyl-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H18 N2 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

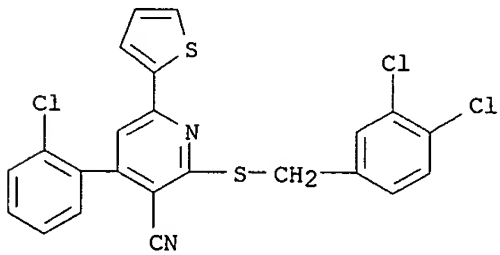
L4 ANSWER 47 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 404919-65-9 REGISTRY
CN 4H-Naphtho[1,2-b]pyran-4-one, 2,3-dihydro-2-[4-methoxy-3-[(2-pyridinylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H21 N O3 S
SR Chemical Library
LC STN Files: CHEMCATS





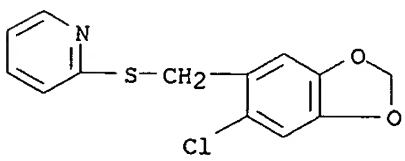
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 48 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 400737-74-8 REGISTRY
CN 3-Pyridinecarbonitrile, 4-(2-chlorophenyl)-2-[[(3,4-dichlorophenyl)methyl]thio]-6-(2-thienyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H13 Cl3 N2 S2
SR Chemical Library



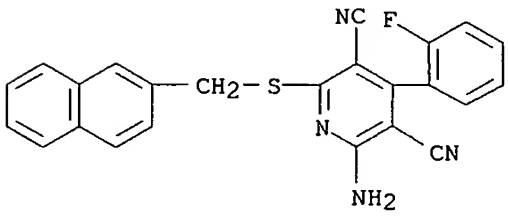
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 49 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 393126-92-6 REGISTRY
CN Pyridine, 2-[[(6-chloro-1,3-benzodioxol-5-yl)methyl]thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H10 Cl N O2 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 50 OF 50 REGISTRY COPYRIGHT 2004 ACS on STN
RN 391667-21-3 REGISTRY
CN 3,5-Pyridinedicarbonitrile, 2-amino-4-(2-fluorophenyl)-6-[(2-naphthalenylmethyl)thio]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H15 F N4 S
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	93.96	94.17

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l4
L5 10 L4

=> d l5 1-10

L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:133263 CAPLUS
DN 138:170241
TI Preparation of benzazepine derivatives as CCR5 antagonists
IN Shiraishi, Mitsuru; Baba, Masanori; Seto, Masaki; Aramaki, Yoshio; Kanzaki, Naoyuki; Miyamoto, Naoki; Iizawa, Yuji
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 584 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003014110	A1	20030220	WO 2002-JP8045	20020807
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2003119191	A2	20030423	JP 2002-229553	20020807

PRAI JP 2001-240718 A 20010808
OS MARPAT 138:170241
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:117800 CAPLUS
DN 138:153442
TI Preparation of heteroarylheteroalkylamines as inhibitors of nitric oxide synthase
IN Birkinshaw, Timothy; Cheshire, David; Connolly, Stephen; Luker, Timothy; Mete, Antonio
PA Astrazeneca AB, Swed.
SO PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003011830	A1	20030213	WO 2002-SE1413	20020726
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI SE 2001-2641 A 20010731
OS MARPAT 138:153442
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:974259 CAPLUS
DN 138:33310
TI Antiretroviral compounds and compositions
IN Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweyko, Arthur M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise Jones Howard L.; Harrison, William A.
PA Uniroyal Chemical Company, Inc., USA
SO U.S., 19 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6498254	B1	20021224	US 2001-21202	20011029
	WO 2003037866	A1	20030508	WO 2002-US29573	20020917

W: AU, BR, CA, CN, JP, MX

PRAI US 2001-21202 A 20011029
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:868910 CAPLUS
DN 137:352896
TI Preparation of arylheteroalkylamine derivatives as nitric oxide synthase inhibitors useful as anti-inflammatories and analgesics
IN Birkinshaw, Tim; Connolly, Stephen; Luker, Timothy; Mete, Antonio; Millichip, Ian
PA Astrazeneca AB, Swed.
SO PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002090332	A2	20021114	WO 2002-SE876	20020506

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI SE 2001-1617 A 20010508
SE 2001-3271 A 20010928
OS MARPAT 137:352896

L5 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:834242 CAPLUS
DN 139:26483
TI Lipophilicity characterization by reversed-phase HPLC of potential antituberculotics
AU Kastner, Petr; Klimes, Jiri; Velenovska, Petra; Klimesova, Vera
CS Faculty of Pharmacy in Hradec Kralove, Charles University in Prague, Hradec Kralove, 500 05, Czech Rep.

SO Journal of Liquid Chromatography & Related Technologies (2002), 25(18), 2849-2856
CODEN: JLCTFC; ISSN: 1082-6076
PB Marcel Dekker, Inc.
DT Journal
LA English
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:805644 CAPLUS
DN 138:201546
TI Pyridine oxide derivatives: Structure-activity relationship for inhibition of human immunodeficiency virus and cytomegalovirus replication in cell culture
AU Balzarini, Jan; Stevens, Miguel; Andrei, Graciela; Snoeck, Robert; Strunk, Richard; Pierce, James B.; Lacadie, John A.; De Clercq, Erik; Pannecouque, Christophe
CS Rega Institute for Medical Research, Katholicke Universiteit Leuven, Louvain, B-3000, Belg.
SO Helvetica Chimica Acta (2002), 85(9), 2961-2975
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:695954 CAPLUS
DN 137:216880
TI Preparation of 2-thio-3,5-dicyano-4-aryl-6-aminopyridines as adenosine receptor-selective ligands
IN Rosentreter, Ulrich; Kraemer, Thomas; Vaupel, Andrea; Huebsch, Walter; Diedrichs, Nicole; Krahn, Thomas; Dembowsky, Klaus; Stasch, Johannes-Peter
PA Bayer Aktiengesellschaft, Germany
SO PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002070485	A1	20020912	WO 2002-EP2121	20020228
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10110754	A1	20020919	DE 2001-10110754	20010307
	EP 1368319	A1	20031210	EP 2002-702377	20020228
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	DE 2001-10110754	A	20010307		
	WO 2002-EP2121	W	20020228		

OS MARPAT 137:216880
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:695053 CAPLUS
DN 138:153519
TI Tributylphosphine-catalyzed acylation of alcohol by active ester directed toward effective end-capping of pseudorotaxane consisting of ammonium group and crown ether
AU Kihara, Nobuhiro; Nakakoji, Naohisa; Takata, Toshikazu
CS Department of Applied Chemistry, Graduate School of Engineering, Osaka Prefecture University, Osaka, 599-8531, Japan
SO Chemistry Letters (2002), (9), 924-925
CODEN: CMLTAG; ISSN: 0366-7022
PB Chemical Society of Japan
DT Journal
LA English
OS CASREACT 138:153519
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:229584 CAPLUS
DN 136:401835
TI Studies toward the Synthesis of .alpha.-Fluorinated Phosphonates via Tin-Mediated Cleavage of .alpha.-Fluoro-.alpha.-(pyrimidin-2-ylsulfonyl)alkylphosphonates. Intramolecular Cyclization of the .alpha.-Phosphonyl Radicals
AU Wnuk, Stanislaw F.; Bergolla, Luis A.; Garcia, Pedro I., Jr.
CS Department of Chemistry, Florida International University, Miami, FL, 33199, USA
SO Journal of Organic Chemistry (2002), 67(9), 3065-3071
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 136:401835
RE.CNT 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:72052 CAPLUS
DN 136:118474
TI Preparation of dicyanopyridine derivatives as high-conductance calcium-sensitive potassium channel openers
IN Harada, Hironori; Watanuki, Susumu; Takuwa, Tomofumi; Kawaguchi, Kenichi; Okazaki, Toshio; Hirano, Yuusuke; Saitoh, Chikashi
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002006237	A1	20020124	WO 2001-JP6136	20010716

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,

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             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     AU 2001069529     A5   20020130       AU 2001-69529    20010716
     EP 1302463        A1   20030416       EP 2001-948028   20010716
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     US 2003232860     A1   20031218       US 2003-333264   20030117
PRAI JP 2000-216982    A    20000718
     WO 2001-JP6136    W    20010716
OS   MARPAT 136:118474
RE.CNT  12    THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> d l5 3 all

L5   ANSWER 3 OF 10  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:974259  CAPLUS
DN   138:33310
ED   Entered STN:  26 Dec 2002
TI   Antiretroviral compounds and compositions
IN   Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweyko, Arthur
     M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise
     Jones Howard L.; Harrison, William A.
PA   Uniroyal Chemical Company, Inc., USA
SO   U.S., 19 pp.
     CODEN: USXXAM
DT   Patent
LA   English
IC   ICM  A61K031-47
     ICS  C07D215-16; C07D211-72; C07D211-84
NCL  546157000; 546290000; 546294000; 514312000; 514345000; 514347000
CC   1-5 (Pharmacology)
     Section cross-reference(s): 27
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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PI   US 6498254         B1   20021224       US 2001-21202    20011029
     WO 2003037866      A1   20030508       WO 2002-US29573  20020917
         W:  AU, BR, CA, CN, JP, MX
PRAI US 2001-21202      A    20011029
AB   Certain pyridine and quinoline derivs. which inhibit replication of the
     retroviruses HIV-1, HIV-2 and human cytomegalovirus (HCMV) are provided.
     Pharmaceutical compns. useful in methods of treating or inhibiting certain
     retrovirus infections are described.
ST   antiretroviral compd pyridine quinoline deriv
IT   Anti-AIDS agents
     Antiviral agents
     Human
     Human herpesvirus 5
     Human immunodeficiency virus 1
     Human immunodeficiency virus 2
        (antiretroviral compds. and compns. using pyridine and quinoline
        derivs.)
IT   Drug delivery systems
        (carriers; antiretroviral compds. and compns. using pyridine and
        quinoline derivs.)
IT   478620-19-8P   478620-24-5P   478620-25-6P   478620-28-9P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (antiretroviral compds. and compns. using pyridine and quinoline
```

derivs.)
IT 69212-31-3P, 2-Benzylthio-3-nitropyridine 478619-45-3P 478619-49-7P
478619-53-3P 478619-57-7P 478619-61-3P 478619-65-7P 478619-68-0P
478619-72-6P 478619-78-2P 478619-82-8P 478619-86-2P 478619-90-8P
478619-94-2P 478619-98-6P 478620-02-9P 478620-06-3P 478620-08-5P
478620-11-0P 478620-12-1P 478620-14-3P 478620-16-5P 478620-18-7P
478620-20-1P 478620-21-2P 478620-23-4P 478620-26-7P 478620-27-8P
478620-29-0P 478620-30-3P 478620-31-4P 478620-32-5P 478620-33-6P
478620-34-7P 478620-35-8P 478620-36-9P 478620-37-0P 478620-38-1P
478620-39-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(antiretroviral compds. and compns. using pyridine and quinoline
derivs.)
IT 51-79-6, Urethane 86-81-7, 3,4,5-Trimethoxybenzaldehyde 100-44-7,
Benzyl chloride, reactions 100-52-7, Benzaldehyde, reactions 100-53-8,
Benzylmercaptan 123-11-5, 4-Methoxybenzaldehyde, reactions 607-66-9,
2-Hydroxy-4-methylquinoline 824-45-3, 2,5-Dimethylbenzyl chloride
2014-83-7, 2,6-Dichlorobenzyl chloride 2044-27-1, 1-Methyl-2(1H)-
pyridinethione 2587-00-0, 2,6-Dichloropyridine-N-oxide 2637-34-5,
2-Mercaptopyridine 3811-73-2 5470-18-8, 2-Chloro-3-nitropyridine
6258-60-2, 4-Methoxybenzylmercaptan 20871-93-6 22182-98-5
52694-50-5, 3-Chloromethyl-1-methylpiperidine 53976-62-8 53976-65-1
60263-88-9 82959-54-4 84504-48-3 91668-83-6, 2-Chloro-3-
methylpyridine-N-oxide 338778-95-3 478619-47-5 478619-51-1
478619-55-5 478619-59-9 478619-63-5 478619-70-4
478619-76-0 478619-80-6 478619-84-0 478619-88-4 478619-92-0
478619-96-4 478620-00-7 478620-05-2 478620-07-4 478620-09-6
478620-10-9 478620-13-2 478620-15-4 478620-17-6 478620-22-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(antiretroviral compds. and compns. using pyridine and quinoline
derivs.)
IT 4437-65-4P 81167-65-9P 81167-66-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(antiretroviral compds. and compns. using pyridine and quinoline
derivs.)
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Brouwer; US 5696151 A 1997 CAPLUS
(2) Harrison; US 5268389 A 1993 CAPLUS
(3) Moormann; US 5945425 A 1999 CAPLUS

=> d his

(FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004
L1 STRUCTURE UPLOADED
L2 0 S L1 EXA SAM
L3 0 S L1 FAM SAM
L4 50 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
L5 10 S L4

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 16.53 110.70

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                  -0.69      -0.69

FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004
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STRUCTURE FILE UPDATES:   20 JAN 2004  HIGHEST RN 639777-15-4
DICTIONARY FILE UPDATES:  20 JAN 2004  HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d his

     (FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

     FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004
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L3            0 S L1 FAM SAM
L4           50 S L1 SSS SAM

     FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
L5           10 S L4

     FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004

=> s l1 sss full
FULL SEARCH INITIATED 09:32:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  11171 TO ITERATE

100.0% PROCESSED   11171 ITERATIONS                          4073 ANSWERS
SEARCH TIME: 00.00.01

L6         4073 SEA SSS FUL L1

=> s hiv or retroviral or retrovirus
            653 HIV
            162 RETROVIRAL
           2918 RETROVIRUS
L7         3719 HIV OR RETROVIRAL OR RETROVIRUS

=> s herpes or herpetic or hsv or hcmv or cmv or hhv
           2328 HERPES
              0 HERPETIC
             26 HSV
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             7 HCMV
            62 CMV
             0 HHV
L8        2422 HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   196.55     307.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -0.69

FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004
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FILE COVERS 1907 - 21 Jan 2004  VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004  (20040120/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s hiv or retroviral or retrovirus
         52913 HIV
         14315 RETROVIRAL
         11976 RETROVIRUS
L9       70667 HIV OR RETROVIRAL OR RETROVIRUS

=> s herpes or herpetic or hsv or hcmv or cmv or hhv
         22109 HERPES
           849 HERPETIC
          9988 HSV
          2423 HCMV
          5770 CMV
          1166 HHV
L10      31317 HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

=> d his

     (FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

     FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004
L1              STRUCTURE UPLOADED
L2            0 S L1 EXA SAM
L3            0 S L1 FAM SAM
L4           50 S L1 SSS SAM
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     FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
L5           10 S L4

     FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004
L6         4073 S L1 SSS FULL
L7         3719 S HIV OR RETROVIRAL OR RETROVIRUS
L8         2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

     FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004
L9        70667 S HIV OR RETROVIRAL OR RETROVIRUS
L10       31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

=> s l6
L11         636 L6

=> s l11 and l9
L12           9 L11 AND L9

=> d l12 1-9

L12  ANSWER 1 OF 9  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:356233  CAPLUS
DN   138:368768
TI   Method for treating human immunodeficiency virus (HIV),
     cytomegalovirus, (HCMV), and herpes virus (HHV) retroviral
     infections by administration of heteroarenes.
IN   Lacadie, John A.; Pierce, James
PA   Uniroyal Chemical Company, Inc., USA
SO   PCT Int. Appl., 57 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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PI   WO 2003037311      A2   20030508       WO 2002-US31836  20021003
     WO 2003037311      A3   20031016
         W:  AU, BR, CA, CN, JP, MX
     US 2003139445      A1   20030724       US 2001-21453    20011029
PRAI US 2001-21453      A    20011029
OS   MARPAT 138:368768

L12  ANSWER 2 OF 9  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:974259  CAPLUS
DN   138:33310
TI   Antiretroviral compounds and compositions
IN   Brewer, Arthur D.; Cantor, Stephen E.; Dekeyser, Mark A.; Doweyko, Arthur
     M. P.; Harris, John W.; Lacadie, John A.; Pierce, James B.; Mary, Louise
     Jones Howard L.; Harrison, William A.
PA   Uniroyal Chemical Company, Inc., USA
SO   U.S., 19 pp.
     CODEN: USXXAM
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
PI   US 6498254         B1   20021224       US 2001-21202    20011029
     WO 2003037866      A1   20030508       WO 2002-US29573  20020917
         W:  AU, BR, CA, CN, JP, MX
PRAI US 2001-21202      A    20011029
RE.CNT  3     THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
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ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:805644 CAPLUS
DN 138:201546
TI Pyridine oxide derivatives: Structure-activity relationship for inhibition of human immunodeficiency virus and cytomegalovirus replication in cell culture
AU Balzarini, Jan; Stevens, Miguel; Andrei, Graciela; Snoeck, Robert; Strunk, Richard; Pierce, James B.; Lacadie, John A.; De Clercq, Erik; Pannecouque, Christophe
CS Rega Institute for Medical Research, Katholicke Universiteit Leuven, Louvain, B-3000, Belg.
SO Helvetica Chimica Acta (2002), 85(9), 2961-2975
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:695955 CAPLUS
DN 137:232650
TI Preparation of nitrogen-containing heteroaryl compounds having **HIV** integrase inhibitory activity
IN Fuji, Masahiro; Mikamiyama, Hidenori; Murai, Hitoshi
PA Shionogi & Co., Ltd., Japan
SO PCT Int. Appl., 316 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002070486	A1	20020912	WO 2002-JP1778	20020227
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1375486	A1	20040102	EP 2002-701583	20020227
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	JP 2001-57037	A	20010301		
	JP 2001-243530	A	20010810		
	JP 2001-395022	A	20011226		
	WO 2002-JP1778	W	20020227		

OS MARPAT 137:232650
RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:784381 CAPLUS
DN 133:335153
TI Preparation of N-arylmethylthioanilide compounds useful for the inhibition of the replication of **HIV**
IN Brouwer, Walter Gerhard; Osika, Ewa Maria

PA Uniroyal Chemical Co., Inc., USA; Uniroyal Chemical Co./cie.
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6143780	A	20001107	US 1999-398649	19990917
WO 2001019811	A2	20010322	WO 2000-US24986	20000912
WO 2001019811	A3	20010726		
W: CA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1220848	A2	20020710	EP 2000-963380	20000912
EP 1220848	B1	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 254611	E	20031215	AT 2000-963380	20000912
PRAI US 1999-398649	A	19990917		
WO 2000-US24986	W	20000912		

OS MARPAT 133:335153
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:705001 CAPLUS
DN 131:322530
TI Substituted tetronic acids useful for treating **HIV** and other retroviruses
IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin, James M.; Smith, Clark W.; Tommasi, Ruben A.; Aristoff, Paul A.; Skulnick, Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.
PA USA
SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 238,820, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5977169	A	19991102	US 1997-604937	19970728
ZA 9406099	A	19960212	ZA 1994-6099	19940812
WO 9507901	A1	19950323	WO 1994-US9533	19940907
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
PRAI US 1993-123029		19930917		
US 1994-238820		19940506		
WO 1994-US9533		19940907		

OS MARPAT 131:322530
RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:585082 CAPLUS
DN 131:331727
TI Structure Based Prediction of Binding Affinity of Human Immunodeficiency Virus-1 Protease Inhibitors

AU Kulkarni, Santosh S.; Kulkarni, Vithal M.
CS Pharmaceutical Division Department of Chemical Technology, University of Mumbai, Matunga Mumbai, 400 019, India
SO Journal of Chemical Information and Computer Sciences (1999), 39(6), 1128-1140
CODEN: JCISD8; ISSN: 0095-2338
PB American Chemical Society
DT Journal
LA English
RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:165733 CAPLUS
DN 126:258470
TI Synthesis and pharmacological evaluation of sulfone substituted **HIV** protease inhibitors
AU Schwartz, Theresa M.; Bundy, Gordon L.; Strohbach, Joseph W.; Thairrivongs, Suvit; Johnson, Paul D.; Skulnick, Harvey I.; Tomich, Paul K.; Lynn, Janet C.; Chong, Kong Teck; Hinshaw, Roger R.; Raub, Thomas J.; Padbury, Guy E.; Loth, Lisa N.
CS Res. Labs., Pharmacia Upjohn, Inc., Kalamazoo, MI, 49001-0199, USA
SO Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 399-402
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier
DT Journal
LA English
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:648144 CAPLUS
DN 123:55683
TI Substituted tetronic acids useful for treating **HIV** and other retroviruses
IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin, James M.; Smith, Clark W.; Tommasi, Rubin A.; Aristoff, Paul A.; Skulnick, Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.
PA Upjohn Co., USA
SO PCT Int. Appl., 223 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9507901	A1	19950323	WO 1994-US9533	19940907
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	CA 2168757	AA	19950323	CA 1994-2168757	19940907
	AU 9476368	A1	19950403	AU 1994-76368	19940907
	EP 720607	A1	19960710	EP 1994-926571	19940907
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09502713	T2	19970318	JP 1994-509195	19940907
	US 5977169	A	19991102	US 1997-604937	19970728
PRAI	US 1993-123029		19930917		
	US 1994-238820		19940506		

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     WO 1994-US9533          19940907
OS   MARPAT 123:55683


=> d l12 9 all

L12  ANSWER 9 OF 9  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1995:648144  CAPLUS
DN   123:55683
ED   Entered STN:  01 Jul 1995
TI   Substituted tetronic acids useful for treating HIV and other
     retroviruses
IN   Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin,
     James M.; Smith, Clark W.; Tommasi, Rubin A.; Aristoff, Paul A.; Skulnick,
     Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.
PA   Upjohn Co., USA
SO   PCT Int. Appl., 223 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  C07D307-60
     ICS  A61K031-365; C07D307-94; C07D405-06; C07D405-12; C07D491-10
CC   27-6 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 1
FAN.CNT 2
     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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             MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US,
             UZ, VN
         RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC,
             NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
     ZA 9406099          A    19960212       ZA 1994-6099      19940812
     CA 2168757          AA   19950323       CA 1994-2168757   19940907
     AU 9476368          A1   19950403       AU 1994-76368     19940907
     EP 720607           A1   19960710       EP 1994-926571    19940907
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
     JP 09502713         T2   19970318       JP 1994-509195    19940907
     US 5977169          A    19991102       US 1997-604937    19970728
PRAI US 1993-123029             19930917
     US 1994-238820             19940506
     WO 1994-US9533             19940907
OS   MARPAT 123:55683
GI
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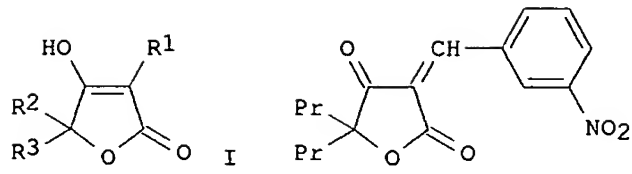
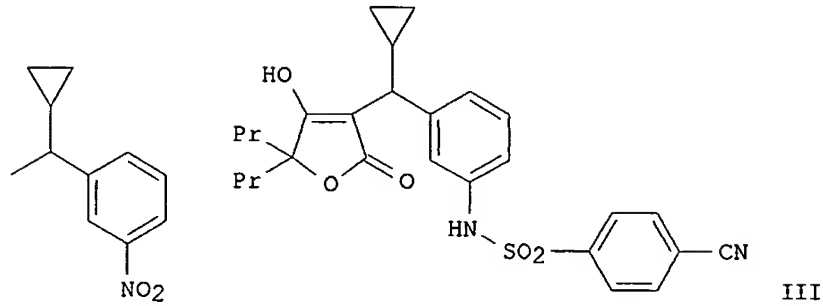


Q1=



AB The invention comprises novel substituted tetronic acid derivs. I and tautomers [wherein R1-R3 = wide variety of specified C-contg. substituents]. I are inhibitors of **HIV** protease, and may be useful for treatment of AIDS or AIDS-related diseases. I may also be used to retard replication of any **retrovirus** contg. aspartyl protease. Approx. 250 compds. are claimed, and phys. and biol. data for approx. 115 compds. are provided. For example, condensation of I [R1 = H, R2 = R3 = Pr] with 3-nitrobenzaldehyde gave >100% crude nitrobenzylidene deriv. II, which reacted with cyclopropylmagnesium bromide and CuBr.SMe2 in THF to give 62% I [R1 = Q1, R2 = R3 = Pr]. Hydrogenation of the nitro group (97%) and sulfonamidation of the resultant amino group with 4-cyanobenzenesulfonyl chloride (53%) gave title compd. III, a preferred compd. Several compds. including III are said to have inhibited replication of **HIV**-1IIIB in human cell lines. **HIV**-1 protease inhibitory data are provided.

ST tetronic acid prepn antiviral **retrovirus**; furandione prepn antiviral **retrovirus**; **HIV** protease inhibitor tetronic acid prepn

IT Virucides and Virustats
(prepn. of antiretroviral tetronic acid derivs.)

IT Acquired immune deficiency syndrome
(treatment; prepn. of antiretroviral tetronic acid derivs.)

IT Virus, animal
(human immunodeficiency, inhibition; prepn. of antiretroviral tetronic acid derivs.)

IT Virus, animal
(human immunodeficiency 1, inhibition; prepn. of antiretroviral tetronic acid derivs.)

IT 144114-21-6, Retropepsin
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(inhibitors of **HIV**; prepn. of antiretroviral tetronic acid derivs.)

IT 78169-47-8, Aspartyl protease
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(inhibitors; prepn. of antiretroviral tetronic acid derivs.)

IT 1138-44-9P 10424-93-8P 72036-34-1P 85520-35-0P 129042-95-1P
161720-04-3P 164344-89-2P 164344-98-3P 164345-52-2P 164346-90-1P
164346-91-2P 164346-92-3P 164346-93-4P 164346-94-5P 164346-95-6P

164346-96-7P 164346-98-9P 164346-99-0P 164347-00-6P 164347-01-7P
164347-02-8P 164347-03-9P 164347-04-0P 164347-07-3P 164347-08-4P
164347-09-5P 164347-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of antiretroviral tetronic acid derivs.)

IT 164344-46-1P 164344-47-2P 164344-48-3P 164344-49-4P 164344-50-7P
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164344-56-3P 164344-57-4P 164344-58-5P 164344-59-6P 164344-60-9P
164344-61-0P 164344-62-1P 164344-63-2P 164344-64-3P 164344-65-4P
164344-66-5P 164344-67-6P 164344-68-7P 164344-69-8P 164344-70-1P
164344-71-2P 164344-72-3P 164344-73-4P 164344-74-5P 164344-75-6P
164344-76-7P 164344-77-8P 164344-78-9P 164344-79-0P 164344-80-3P
164344-81-4P 164344-82-5P 164344-83-6P 164344-84-7P 164344-85-8P
164344-86-9P 164344-87-0P 164344-88-1P 164344-89-2P 164344-90-5P
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164345-21-5P 164345-22-6P 164345-23-7P 164345-24-8P 164345-25-9P
164345-26-0P 164345-27-1P 164345-28-2P 164345-29-3P 164345-30-6P
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164346-42-3P 164346-43-4P 164346-44-5P **164346-45-6P**
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164346-50-3P 164346-51-4P 164346-52-5P 164346-53-6P 164346-54-7P
164346-55-8P 164346-56-9P **164346-57-0P 164346-58-1P**
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164346-63-8P 164346-64-9P 164346-65-0P 164346-66-1P 164346-67-2P
164346-68-3P **164346-69-4P 164346-70-7P**
164346-71-8P 164346-72-9P 164346-73-0P 164346-74-1P
164346-75-2P 164346-76-3P 164346-77-4P 164346-78-5P 164346-79-6P
164346-80-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of antiretroviral tetronic acid derivs.)

IT **164346-81-0P 164346-82-1P 164346-83-2P**
164346-84-3P 164346-85-4P 164346-86-5P 164346-87-6P 164346-88-7P
164346-89-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of antiretroviral tetronic acid derivs.)

IT 57-14-7, 1,1-Dimethylhydrazine 74-96-4, Bromoethane 99-61-6, 3-Nitrobenzaldehyde 100-39-0, Benzyl bromide 103-63-9, (2-Bromoethyl)benzene 104-53-0, Hydrocinnamaldehyde 106-94-5, Propyl bromide 108-94-1, Cyclohexanone, reactions 120-92-3, Cyclopentanone 123-19-3, 4-Heptanone 501-53-1, Benzyl chloroformate 502-49-8, Cyclooctanone 623-47-2, Ethyl propiolate 637-59-2, 1-Bromo-3-phenylpropane 946-33-8, 2-Benzylcyclohexanone 1007-03-0, .alpha.-Cyclopropylbenzyl alcohol 1067-74-9, Methyl diethylphosphonoacetate 1138-44-9 2550-26-7, Benzyl acetone 2637-37-8, 2-Quinolinethiol 4423-94-3, 2-Ethylcyclohexanone 4971-56-6, Tetronic acid 14371-10-9, trans-Cinnamaldehyde 23719-80-4, Cyclopropylmagnesium bromide 28920-43-6, 9-Fluorenylmethyl chloroformate 29976-53-2, 1-Carbethoxy-4-piperidone 49584-26-1, 4-Cyanobenzenesulfonyl chloride 118753-70-1 164345-06-6 164346-97-8 164347-05-1 164347-06-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prepn. of antiretroviral tetronic acid derivs.)

=> d l12 8 all

L12 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:165733 CAPLUS
DN 126:258470
ED Entered STN: 12 Mar 1997
TI Synthesis and pharmacological evaluation of sulfone substituted **HIV** protease inhibitors
AU Schwartz, Theresa M.; Bundy, Gordon L.; Strohbach, Joseph W.; Thairrivongs, Suvit; Johnson, Paul D.; Skulnick, Harvey I.; Tomich, Paul K.; Lynn, Janet C.; Chong, Kong Teck; Hinshaw, Roger R.; Raub, Thomas J.; Padbury, Guy E.; Loth, Lisa N.
CS Res. Labs., Pharmacia Upjohn, Inc., Kalamazoo, MI, 49001-0199, USA
SO Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 399-402
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier
DT Journal
LA English
CC 1-3 (Pharmacology)
AB The sulfonamide substituted pyranones (1) have recently been shown to be potent **HIV** protease inhibitors. We prepard a series of sulfone substituted analogs and compared and their biol. activities to those of the corresponding sulfonamide analogs. It was detd. that although these compds. maintained activity as enzyme inhibitors, they showed somewhat diminished antiviral activity event though they may possess increased membrane permeability.
ST sulfonamide pyranone prepn **HIV** protease inhibitor
IT Structure-activity relationship
(antiviral; sulfonamide substituted pyranones as **HIV** protease inhibitors)
IT Structure-activity relationship
(aspartic proteinase-inhibiting; sulfonamide substituted pyranones as **HIV** protease inhibitors)
IT Anti-AIDS agents
Antiviral agents
Human immunodeficiency virus 1
(sulfonamide substituted pyranones as **HIV** protease inhibitors)
IT 174483-90-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antiviral and **HIV**-1 protease inhibiting activity of)

IT 166335-18-8P 166335-24-6P 166335-32-6P 166335-74-6P 166335-80-4P
174483-25-1P 174483-26-2P 174483-27-3P 174483-28-4P 174483-29-5P
174483-30-8P 174483-56-8P 174483-62-6P 174483-63-7P 174483-94-4P
188839-13-6P 188839-14-7P 188839-15-8P **188839-16-9P**
188839-17-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antiviral and **HIV**-1 protease inhibiting activity of)

IT 162174-73-4P 174484-94-7P 188839-19-2P 188839-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of)

IT 675-10-5 7051-34-5, Bromomethyl cyclopropane 100058-82-0 174484-93-6
188839-18-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	36.86	344.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.39	-2.08

FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4
DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> S 188839-16-9/RN

L13 1 188839-16-9/RN

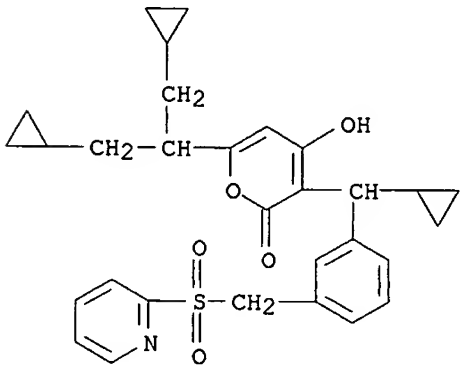
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L13 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 5.92 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN **188839-16-9** REGISTRY
CN 2H-Pyran-2-one, 6-[2-cyclopropyl-1-(cyclopropylmethyl)ethyl]-3-[cyclopropyl[3-[(2-pyridinylsulfonyl)methyl]phenyl]methyl]-4-hydroxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H33 N O5 S
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> d l12 7 all
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:n

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.61	346.72

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.08

FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l12 7 all

L12 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:585082 CAPLUS
DN 131:331727
ED Entered STN: 20 Sep 1999
TI Structure Based Prediction of Binding Affinity of Human Immunodeficiency Virus-1 Protease Inhibitors
AU Kulkarni, Santosh S.; Kulkarni, Vithal M.
CS Pharmaceutical Division Department of Chemical Technology, University of Mumbai, Matunga Mumbai, 400 019, India
SO Journal of Chemical Information and Computer Sciences (1999), 39(6), 1128-1140
CODEN: JCISD8; ISSN: 0095-2338
PB American Chemical Society
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 7, 22
AB A series of computations were performed to derive a strategy for the prediction of binding affinities of non-peptidic human immunodeficiency virus-1 (**HIV**-1) protease inhibitors. This paper describes the development of a 3D quant. structure-activity relation (3D-QSAR) methodol. by using receptor information of **HIV**-1 protease. The docking and mol. dynamics simulations were performed on a model ligand/enzyme complex to optimize the variables involved in the generation of

ligand/enzyme models. The protonation scheme of the active site aspartic acid residues of **HIV**-1 protease was derived from a computational study. The active site aspartate is monoprotonated with a proton placed on the OD1 atom of the ASP B25. This protocol of docking and mol. dynamics (MD) simulation was then used to derive the ligand-enzyme complexes of the mols. used in the present study. The mol. mechanics interaction descriptors were calcd. from these ligand/enzyme models. A partial least squares (PLS) method was used to derive a linear correlation between the interaction descriptors and the biol. activity. A good correlation was obsd. when the change in the energy of the ligand upon complex formation and the electrostatic contributions to the solvation energy of the ligand were included in the QSAR anal. A highest cross-validated q2 value of 0.649 was obsd. This model had a conventional r2 of 0.725, and when this model was used to predict the activity of the external test set, it produced a r2pred of 0.761. The total interaction energy was partitioned into interactions in different subsites and interactions with each of the amino acid residues of the enzyme. The PLS anal. using these descriptors helped to identify the important interactions which can be exploited for the design of **HIV**-1 protease inhibitors.

ST HIV1 virus protease inhibitor QSAR design; drug design HIV1 virus protease inhibitor

IT Enzyme functional sites
(active; structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT Simulation and Modeling, biological
(mol. dynamics; structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT Conformation
Human immunodeficiency virus 1
Molecular association
Molecular modeling
Potential energy
QSAR (structure-activity relationship)
(structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT 81-81-2 435-97-2 149394-65-0 158200-29-4 162168-60-7 162168-64-1
162168-92-5 162169-60-0 162169-80-4 162169-86-0 163020-86-8
163020-88-0 163020-92-6 163021-01-0 163021-02-1 166186-75-0
166186-77-2 166282-31-1 166282-37-7 166282-99-1 166334-73-2
166334-76-5 166334-90-3 166335-18-8 166335-74-6 174483-57-9
174483-59-1 174483-62-6 174484-41-4 174484-42-5 174484-53-8
174484-54-9 176771-70-3 183963-05-5 183964-16-1 **188839-16-9**
188839-17-0 213014-48-3 249765-76-2 249765-77-3
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

IT 144114-21-6, Retropepsin
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(structure based prediction of binding affinity of human immunodeficiency virus-1 protease inhibitors)

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD

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=> d l12 6 all

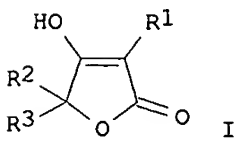
L12 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:705001 CAPLUS
DN 131:322530
ED Entered STN: 04 Nov 1999
TI Substituted tetronic acids useful for treating **HIV** and other retroviruses
IN Chrusciel, Robert A.; Maggiora, Linda L.; Thaisrivongs, Suvit; Tustin, James M.; Smith, Clark W.; Tommasi, Ruben A.; Aristoff, Paul A.; Skulnick, Harvey I.; Howe, W. Jeffrey; Bundy, Gordon L.
PA USA
SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 238,820, abandoned.
CODEN: USXXAM

DT Patent
LA English
IC ICM A61K031-34
ICS A61K031-335; A61K031-415; A61K031-505
NCL 514473000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5977169	A	19991102	US 1997-604937	19970728
	ZA 9406099	A	19960212	ZA 1994-6099	19940812
	WO 9507901	A1	19950323	WO 1994-US9533	19940907

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

PRAI US 1993-123029 19930917
US 1994-238820 19940506
WO 1994-US9533 19940907
OS MARPAT 131:322530
GI



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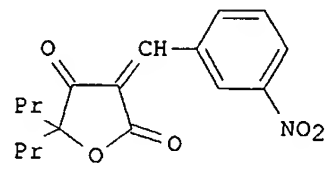
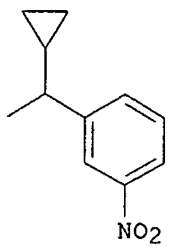
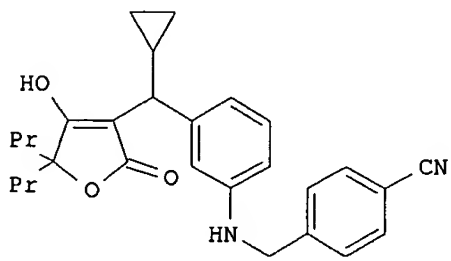


II

Q1=





III

AB The invention comprises novel substituted tetronic acid derivs. (I) and tautomers [wherein R1-R3 = wide variety of specified C-contg. substituents] that are inhibitors of **HIV** protease. I retard replication of any **retrovirus** contg. aspartyl protease and are useful for treatment of AIDS or AIDS-related diseases. Approx. 250 compds. are claimed, and phys. and biol. data for approx. 120 compds. are provided. For example, condensation of I [R1 = H, R2 = R3 = Pr] with 3-nitrobenzaldehyde gave >100% crude nitrobenzylidene deriv. II, which reacted with cyclopropylmagnesium bromide and CuBr.SMe2 in THF to give 62% I [R1 = Q1, R2 = R3 = Pr]. Hydrogenation of the nitro group (97%) and sulfonamidation of the resultant amino group with 4-cyanobenzenesulfonyl chloride (53%) gave title furandione III, a preferred compd. Several compds. including III are said to have inhibited replication of **HIV**-1IIIB in human cell lines. **HIV**-1 protease inhibitory data are provided, and over 100% inhibition was reported for

many test compds. at doses as low as 3.3 .mu.M.

ST tetronic acid prepn antiviral **retrovirus** replication inhibitor; furandione prepn antiviral **retrovirus** replication inhibitor; **HIV** protease inhibitor AIDS treatment tetronic acid prepn

IT Human immunodeficiency virus
Human immunodeficiency virus 1
(inhibition; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT Anti-AIDS agents
Antiviral agents
(prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT AIDS (disease)
(treatment; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 144114-21-6, Retropepsin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 1138-44-9P 10424-93-8P 72036-34-1P 85520-35-0P 161720-04-3P
164346-90-1P 164346-91-2P 164346-92-3P 164346-93-4P 164346-94-5P
164346-95-6P 164346-96-7P 164346-98-9P 164346-99-0P 164347-01-7P
164347-02-8P 164347-03-9P 164347-07-3P 164347-10-8P 248608-58-4P
248608-59-5P 248608-60-8P 248608-61-9P 248608-62-0P 248608-63-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 99-61-6, 3-Nitrobenzaldehyde 100-39-0, Benzyl bromide 103-63-9, (2-Bromoethyl)benzene 104-53-0, Hydrocinnamaldehyde 106-94-5 108-94-1, Cyclohexanone, reactions 109-72-8, n-Butyl lithium, reactions 120-92-3, Cyclopentanone 502-49-8, Cyclooctanone 623-47-2, Ethyl propiolate 637-59-2, 1-Bromo-3-phenylpropane 946-33-8, 2-Benzylcyclohexanone 1007-03-0, .alpha.-Cyclopropylbenzyl alcohol 1067-74-9, Methyl diethylphosphonoacetate 2550-26-7, Benzyl acetone 2637-37-8, 2-Quinolinethiol 4423-94-3, 2-Ethylcyclohexanone 4971-56-6, Tetronic acid 14371-10-9 23719-80-4, Cyclopropylmagnesium bromide 29976-53-2, 1-Carbethoxy-4-piperidone 49584-26-1, 4-Cyanobenzenesulfonyl chloride 118753-70-1 135005-10-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 164344-46-1P 164344-47-2P 164344-48-3P 164344-49-4P 164344-50-7P
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164344-66-5P 164344-67-6P 164344-68-7P 164344-69-8P 164344-70-1P
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164344-76-7P 164344-77-8P 164344-79-0P 164344-80-3P 164344-81-4P
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248608-45-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

IT 248608-46-0P 248608-48-2P 248608-49-3P 248608-50-6P 248608-51-7P
248608-52-8P 248608-53-9P 248608-54-0P 248608-56-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compd.; prepn. of antiretroviral tetronic acid derivs. for treatment of AIDS or AIDS-related diseases)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Anderson, J; JCS Perkin 1 1982, V1, P215
(2) Anon
(3) Anon; 1963
(4) Anon; 1965
(5) Anon; 1977 CAPLUS
(6) Anon; 1979 CAPLUS
(7) Anon; 1979 CAPLUS
(8) Anon; 1979 CAPLUS
(9) Anon; 1982 CAPLUS
(10) Anon; 1983 CAPLUS
(11) Anon; EP 0202589 A2 1986 CAPLUS
(12) Anon; EP 0259707 1988 CAPLUS
(13) Anon; EP 0365329 1990 CAPLUS
(14) Anon; JP 04-211676 1992 CAPLUS
(15) Anon; EP 0480624 A1 1992 CAPLUS
(16) Anon; 1993 CAPLUS
(17) Anon; JP 05-043568 1993 CAPLUS
(18) Anon; EP 0534907 1993 CAPLUS

(19) Anon; WO 9304055 1993 CAPLUS
(20) Anon; WO 9411361 1994 CAPLUS
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(36) Vekemans, J; Tetrahedron Letters 1987, V28(20), P2299 CAPLUS
(37) Wakabayashi, H; Chemistry Letters 1987, P875
(38) Wanwagenen, B; Tetrahedron 1986, V42(4), P1117

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L12 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:784381 CAPLUS
DN 133:335153
ED Entered STN: 09 Nov 2000
TI Preparation of N-arylmethylthioanilide compounds useful for the inhibition of the replication of **HIV**
IN Brouwer, Walter Gerhard; Osika, Ewa Maria
PA Uniroyal Chemical Co., Inc., USA; Uniroyal Chemical Co./cie.
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-505
ICS A61K031-381; C07D307-68; C07D333-38; C07D405-12
NCL 514471000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 10
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6143780	A	20001107	US 1999-398649	19990917
	WO 2001019811	A2	20010322	WO 2000-US24986	20000912
	WO 2001019811	A3	20010726		
	W: CA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1220848	A2	20020710	EP 2000-963380	20000912
	EP 1220848	B1	20031119		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
	AT 254611	E	20031215	AT 2000-963380	20000912
PRAI	US 1999-398649	A	19990917		
	WO 2000-US24986	W	20000912		

OS MARPAT 133:335153
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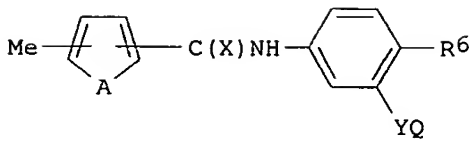

I

AB The title compds. I [A, X are independently O or S; R6 = H, halo, alkyl, alkoxy, alkylthio, cyano, nitro; Y = CH2O, OCH2, CH2S, CH2SO2; Q = substituted or unsubstituted Ph or arom. heterocyclic group], useful for the inhibition of the replication of **HIV**-1 in vitro and in vivo, were prepd. E.g. N-3-((2-chlorophenoxy)methyl)-4-chlorophenyl-2-methyl-3-furancarbothioamide was prepd.

ST arylmethylthioanilide prepn inhibition HIV1; furancarbothioamide prepn inhibition HIV1; furancarboxamide prepn inhibition HIV1

IT Human immunodeficiency virus 1
(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV**-1)

IT 255381-42-1P 303964-42-3P 303964-43-4P 303964-44-5P 303964-45-6P
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303965-16-4P 303965-17-5P 303965-28-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV**-1)

IT 5555-00-0 6361-21-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV**-1)

IT 95-57-8P, 2-Chlorophenol 80866-80-4P 124877-63-0P 303965-18-6P
303965-19-7P 303965-20-0P 303965-21-1P 303965-22-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of N-arylmethylthioanilide compds. useful for the inhibition of the replication of **HIV**-1)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Brouwer; US 5696151 1997 CAPLUS
(2) Brouwer; US 6017947 2000 CAPLUS

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L12 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:695955 CAPLUS
DN 137:232650
ED Entered STN: 13 Sep 2002

TI Preparation of nitrogen-containing heteroaryl compounds having **HIV** integrase inhibitory activity

IN Fuji, Masahiro; Mikamiyama, Hidenori; Murai, Hitoshi
PA Shionogi & Co., Ltd., Japan

SO PCT Int. Appl., 316 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07D215-28
ICS C07D215-48; C07D215-50; C07D235-10; C07D235-08; C07D417-04; C07D417-06; C07D413-04; C07D413-14; C07D491-04; C07D491-048; C07D487-04; C07D513-04; C07D495-04; A61K031-4184; A61K031-427; A61K031-4245; A61K031-422; A61K031-433; A61K031-428
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002070486	A1	20020912	WO 2002-JP1778	20020227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1375486	A1	20040102	EP 2002-701583	20020227
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRAI JP 2001-57037 A 20010301
JP 2001-243530 A 20010810
JP 2001-395022 A 20011226
WO 2002-JP1778 W 20020227
OS MARPAT 137:232650
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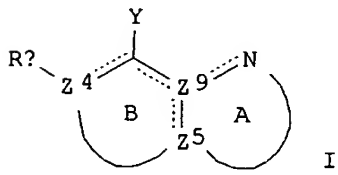

I

AB The title compds. I [rings A and B are fused N-contg. heterocyclic rings; Z4, Z5 and Z9 independently represent each carbon or nitrogen; Y represents hydroxy, mercapto or amino; and RA represents nitrogen-contg. heteroaryl, etc.] are prepd. Compds. of this invention in vitro showed IC50 values of 0.11 .mu.g/mL to 0.76 .mu.g/mL against **HIV** integrase. Formulations are given.

ST heteroaryl compd prepn **HIV** integrase inhibitor

IT Enzymes, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and enzyme inhibitory activity)

IT Salts, preparation
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and salts thereof)

IT Human
Solvates
(prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and solvates thereof)

IT AIDS (disease)
Anti-AIDS agents
(prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT Drug delivery systems
(prodrugs; prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and prodrugs thereof)

IT Nucleic acids
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(related enzymes; prepn. and effect of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and enzyme inhibitory activity)

IT 144114-21-6, **HIV** protease
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(combination of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and protease inhibitors)

IT 9068-38-6, Reverse transcriptase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(combination of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity and reverse transcriptase inhibitors)

IT 52350-85-3, **HIV** integrase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(of **HIV**; prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT 205040-56-8P 410544-61-5P 457945-02-7P 457945-04-9P 457945-05-0P
457945-06-1P 457945-07-2P 457945-08-3P 457945-09-4P 457945-10-7P
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457945-16-3P 457945-17-4P 457945-18-5P 457945-19-6P 457945-20-9P
457945-21-0P 457945-22-1P 457945-23-2P 457945-24-3P 457945-25-4P
457945-26-5P 457945-27-6P 457945-28-7P 457945-29-8P 457945-30-1P
457945-31-2P 457945-32-3P 457945-33-4P 457945-34-5P 457945-35-6P
457945-36-7P 457945-37-8P 457945-38-9P 457945-39-0P 457945-40-3P
457945-41-4P 457945-42-5P 457945-43-6P 457945-44-7P 457945-45-8P
457945-46-9P 457945-47-0P 457945-48-1P 457945-49-2P 457945-50-5P
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457947-39-6P 457947-40-9P 457947-41-0P 457947-42-1P 457947-43-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity).

IT 457947-44-3P 457947-45-4P 457947-46-5P 457947-47-6P 457947-48-7P
457947-49-8P 457947-50-1P 457947-51-2P 457947-52-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT 64-17-5, Ethanol, reactions 74-88-4, Methyl iodide, reactions 74-89-5, Methylamine, reactions 74-96-4, Ethyl bromide 75-07-0, Acetaldehyde, reactions 75-16-1, Methylmagnesium bromide 75-31-0, Isopropylamine, reactions 75-36-5, Acetyl chloride 77-78-1, Dimethyl sulfate 85-38-1 87-13-8, Diethyl ethoxymethylenemalonate 90-04-0, 2-Methoxyaniline 96-33-3, Methyl acrylate 98-80-6, Phenylboronic acid 100-39-0, Benzyl bromide 100-46-9, Benzylamine, reactions 103-72-0, Phenylthioisocyanate 107-21-1, Ethylene glycol, reactions 107-30-2, Methoxymethyl chloride 108-24-7, Acetic anhydride 123-62-6, Propionic anhydride 124-38-9, Carbon dioxide, reactions 124-40-3, Dimethylamine, reactions 124-41-4, Sodium methoxide 288-32-4, Imidazole, reactions 302-01-2, Hydrazine, reactions 334-88-3, Diazomethane 405-50-5, p-Fluorophenylacetic acid 431-03-8, Diacetyl 459-04-1, 4-Fluorophenylacetyl chloride 459-32-5 459-46-1, 4-Fluorobenzyl bromide 462-08-8, 3-Aminopyridine 501-52-0, Benzenepropanoic acid 506-59-2, Dimethylamine hydrochloride 506-68-3, Bromocyanide 521-74-4 544-92-3, Copper cyanide 607-35-2 630-08-0, Carbon monoxide, reactions 824-79-3, Sodium p-toluenesulfinate 937-39-3, Phenylacetylhydrazide 1066-54-2, Trimethylsilylacetylene 1117-97-1, N,O-Dimethylhydroxylamine 1461-22-9, Tributyltin chloride 2127-03-9, 2,2'-Dipyridyldisulfide 2533-69-9, Methyl 2,2,2-trichloroacetimidate 2591-86-8, N-Formylpiperidine 3034-53-5, 2-Bromothiazole 4595-60-2, 2-Bromopyrimidine 4637-24-5, Dimethylformamide dimethylacetal 5419-55-6, Triisopropyl borate 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 7486-35-3, Tributylvinylstannane 7553-56-2, Iodine, reactions 7640-33-7 7664-41-7, Ammonia, reactions 7726-95-6, Bromine, reactions 12125-02-9, Ammonium chloride, reactions 19829-79-9 31230-17-8 34547-28-9 51110-60-2 56826-69-8 64214-66-0 73183-34-3, Bis(pinacolato)diborane 76513-69-4, 2-(Trimethylsilyl)ethoxymethyl chloride 91478-74-9 93102-98-8,

1-Amino-3-(4-fluorophenyl)propan-2-one hydrochloride 107095-99-8
115192-48-8 126463-85-2 126463-87-4 145837-83-8 154355-81-4,
2-Bromo-5-(p-fluorobenzyl)furan 199931-43-6 280572-13-6 457947-54-5
457947-55-6 457947-56-7 457947-57-8 457947-58-9 457947-60-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT 459-31-4P, 4-Fluorobenzenepropanoic acid 5129-25-9P 5341-07-1P
7175-09-9P 14151-06-5P 17012-49-6P 20075-26-7P 63416-70-6P
90564-26-4P 101226-33-9P 103030-27-9P 121359-48-6P 126545-09-3P
130091-84-8P 139399-62-5P 139399-67-0P 146697-85-0P 170959-58-7P
174485-36-0P 223761-28-2P 243145-83-7P 457931-02-1P 457935-27-2P
457947-53-4P 457947-59-0P 457947-61-4P 457947-62-5P 457947-63-6P
457947-65-8P 457947-66-9P 457947-67-0P 457947-68-1P 457947-69-2P
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457949-19-8P 457949-20-1P 457949-21-2P 457949-22-3P 457949-23-4P
457949-24-5P 457949-25-6P 457949-26-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

IT 459476-94-9 459476-95-0 459476-96-1 459476-97-2
RL: PRP (Properties)
(unclaimed sequence; prepn. of nitrogen-contg. heteroaryl compds. having **HIV** integrase inhibitory activity)

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

(1) Centre National de La Recherche Scientifique; JP 2001518890 A 1998
(2) Centre National de La Recherche Scientifique; FR 2761687 A 1998 CAPLUS
(3) Centre National de La Recherche Scientifique; EP 975597 A1 1998 CAPLUS
(4) Centre National de La Recherche Scientifique; WO 9845269 A1 1998 CAPLUS
(5) Fuji Photo Film Co Ltd; JP 05027385 A 1993 CAPLUS
(6) Haworth, I; Anti-Cancer Drug Des 1991, V6(1), P59 CAPLUS

(7) Mekouar, K; J Med Chem 1998, V41(15), P2846 CAPLUS
(8) Merck & Co Inc; WO 0230426 A1 2002 CAPLUS
(9) Merck & Co Inc; WO 0230426 A1 2002 CAPLUS
(10) Merck & Co Inc; WO 0230930 A2 2002 CAPLUS
(11) Merck & Co Inc; US 2002019397 A 2002 CAPLUS
(12) Ouali, M; J Med Chem 2000, V43(10), P1949 CAPLUS
(13) Pharmacia & Upjohn Co; JP 2002505660 A 1998
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(18) Shankar, M; J Indian Chem Society 1982, V59(9), P1104 CAPLUS
(19) Sumitomo Chemical Co; GB 1446484 A 1976 CAPLUS
(20) Sumitomo Chemical Co; GB 1488173 A 1976 CAPLUS
(21) Sumitomo Chemical Co; FR 2210385 A 1976 CAPLUS
(22) Sumitomo Chemical Co; FR 2255898 A 1976 CAPLUS
(23) Sumitomo Chemical Co; DE 2362279 A 1976 CAPLUS
(24) Sumitomo Chemical Co; DE 2461526 A 1976 CAPLUS
(25) Sumitomo Chemical Co; US 3954733 A 1976 CAPLUS
(26) Sumitomo Chemical Co; US 3992371 A 1976 CAPLUS
(27) Sumitomo Chemical Co; JP 49082683 A 1976 CAPLUS
(28) Sumitomo Chemical Co; JP 50096594 A 1976 CAPLUS
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(31) Sumitomo Chemical Co; GB 1532866 A 1978 CAPLUS
(32) Sumitomo Chemical Co; FR 2332758 A 1978 CAPLUS
(33) Sumitomo Chemical Co; US 4125611 A 1978 CAPLUS
(34) Sumitomo Chemical Co; JP 52068193 A 1978 CAPLUS
(35) Sumitomo Chemical Co; AU 7620018 A 1978 CAPLUS
(36) The Department Of Health And Human Services; US 5681832 A 1997 CAPLUS
(37) The Department Of Health And Human Services; WO 9625399 A1 1997 CAPLUS
(38) The Department Of Health And Human Services; AU 9649855 A 1997 CAPLUS
(39) Zouhiri, F; J Med Chem 2000, V43(8), P1533 CAPLUS
(40) Zouhiri, F; Tetrahedron Letters 2001, V42(46), P8189 CAPLUS

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	14.93	361.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.77	-4.85

FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4
DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> S 457949-18-7/RN

L14 1 457949-18-7/RN

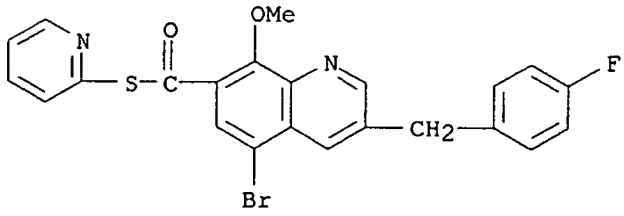
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L14 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 5.92 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN **457949-18-7** REGISTRY
CN 7-Quinolinecarbothioic acid, 5-bromo-3-[(4-fluorophenyl)methyl]-8-methoxy-, S-2-pyridinyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H16 Br F N2 O2 S
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.19	363.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-4.85

FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l11 and l10
L15           5 L11 AND L10

=> s l15 not l12
L16           2 L15 NOT L12

=> d l16 1-2

L16  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1999:561590  CAPLUS
DN   131:184948
TI   Preparation of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase
     inhibitors useful as antiviral agents.
IN   Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil,
     Clara I.
PA   G.D. Searle & Co., USA
SO   U.S., 54 pp., Cont.-in-part of Ser. No. US 1994-
     CODEN: USXXAM
DT   Patent
LA   English
FAN.CNT 2
     PATENT NO.         KIND  DATE           APPLICATION NO.   DATE
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PI   US 5945425          A    19990831       US 1996-737251    19961024
     WO 9529897          A1   19951109       WO 1995-US5021    19950501
         W:  AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,
             GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,
             MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,
             TM, TT
         RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
             SN, TD, TG
     US 2001047038       A1   20011129       US 2001-885221    20010620
PRAI US 1994-235619      B2   19940429
     WO 1995-US5021      W    19950501
     US 1996-659098      B1   19960604
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     US 1999-377888     B1   19990819
     US 2000-605560     B1   20000627
OS   MARPAT 131:184948
RE.CNT  45    THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16  ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1970:111444  CAPLUS
DN   72:111444
TI   Antiviral and neuroleptic .alpha.-carbolines
PA   Glaxo Laboratories Ltd.
SO   Fr. Demande, 52 pp.
     CODEN: FRXXBL
DT   Patent
LA   French
FAN.CNT 1
     PATENT NO.         KIND  DATE          APPLICATION NO.  DATE
     ---------------    ----  --------      ---------------  --------
PI   FR 2003999                 19691114
     DE 1913119                               DE
     GB 1268772                               GB
     ZA 6901818                 19690000      ZA
PRAI GB                         19680315


=> d l16 1 all

L16  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1999:561590  CAPLUS
DN   131:184948
ED   Entered STN:  03 Sep 1999
TI   Preparation of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase
     inhibitors useful as antiviral agents.
IN   Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil,
     Clara I.
PA   G.D. Searle & Co., USA
SO   U.S., 54 pp., Cont.-in-part of Ser. No. US 1994-
     CODEN: USXXAM
DT   Patent
LA   English
IC   ICM  A61K031-42
     ICS  A61K031-415; A61K031-425
NCL  514269000
CC   28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1
FAN.CNT 2
     PATENT NO.         KIND  DATE          APPLICATION NO.  DATE
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PI   US 5945425          A    19990831      US 1996-737251   19961024
     WO 9529897          A1   19951109      WO 1995-US5021   19950501
         W:  AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,
             GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,
             MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,
             TM, TT
         RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
             SN, TD, TG
     US 2001047038       A1   20011129      US 2001-885221   20010620
PRAI US 1994-235619      B2   19940429
     WO 1995-US5021      W    19950501
     US 1996-659098      B1   19960604
     US 1999-377888      B1   19990819
```

US 2000-605560 B1 20000627

OS MARPAT 131:184948

AB A method of treating viral infection comprises treatment with R2(CR3R4)pSOm(CR4R5)nR1 [R1 = (substituted) alkoxy, alkoxycarbonyl, dialkylamino, aryl, heteroaryl; R2 = (substituted) heteroaryl; R3-R6 = H, alkyl, aryl, aralkyl; R3R4, R5R6 = cycloalkyl; m, n, p = 0-2]. Thus, 2-mercaptobenzimidazole and 2-aminobenzyl alc. were heated in HOAc/H2SO4 to give 2-[(1H-benzimidazol-2-yl)thiomethyl]benzeneamine. The latter in CHCl3 was treated with 2-[(1H-benzimidazol-2-yl)sulfinylmethyl]benzeneamin e. Title compds. inhibited **HCMV** replication with EC50 = 13-61 .mu.M.

ST benzimidazolylsulfinylmethylarylamine prepn ATPase inhibitor antiviral

IT Antiviral agents
(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

IT 100924-68-3P 104340-33-2P 104340-34-3P 104340-35-4P 104340-37-6P
104340-38-7P 104524-67-6P 104524-68-7P 106746-58-1P 106746-60-5P
106746-61-6P 106746-63-8P 106746-65-0P 106746-66-1P 106746-68-3P
106746-69-4P 106746-76-3P 106746-77-4P 106746-78-5P 106746-79-6P
106746-80-9P 106746-84-3P 106746-86-5P 106746-88-7P 106746-90-1P
106746-93-4P 106746-94-5P 106746-95-6P 106746-96-7P 106746-97-8P
106746-98-9P 106747-00-6P 106747-05-1P 106747-06-2P 106747-07-3P
106747-08-4P 106747-10-8P 106747-11-9P 106747-12-0P 106747-13-1P
106747-14-2P 106747-15-3P 106747-16-4P 106747-17-5P 106747-18-6P
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106747-29-9P 106747-30-2P 106747-31-3P 106747-32-4P 106747-33-5P
106747-34-6P 106747-35-7P 106747-36-8P 106747-38-0P 106747-39-1P
106747-40-4P 106747-41-5P 106747-42-6P 106747-43-7P 106747-44-8P
106747-45-9P 106747-47-1P 106747-48-2P 106771-58-8P 106785-95-9P
106785-96-0P 108542-64-9P 108542-66-1P 111477-14-6P 111502-75-1P
114060-19-4P 118267-21-3P 118267-22-4P 118267-23-5P 118267-24-6P
118267-25-7P 118267-26-8P 118267-27-9P 118267-28-0P 118267-29-1P
118267-30-4P 118267-33-7P 118267-34-8P 118267-35-9P 118267-36-0P
118267-37-1P 118267-38-2P 118267-39-3P 118267-42-8P 118267-43-9P
118292-92-5P 118292-93-6P 118292-94-7P 118292-95-8P 118292-96-9P
118292-97-0P 118292-98-1P 118292-99-2P 174397-92-3P 174397-93-4P
174397-94-5P 174397-95-6P 174397-96-7P 174397-97-8P 174397-98-9P
174397-99-0P 174398-00-6P 174398-01-7P 174398-02-8P 174398-03-9P
174398-04-0P **174398-05-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

IT 55546-06-0 56713-45-2 57235-18-4 60524-97-2 71670-48-9
73590-36-0 73590-58-6 73590-61-1 81527-04-0 81864-40-6
81864-65-5 94452-40-1 96733-60-7 96831-93-5 97288-52-3
97963-93-4 97966-85-3 98412-35-2 98412-41-0 99153-80-7
99499-40-8 101387-97-7 102127-07-1 102127-11-7 102625-54-7
102625-70-7 102625-79-6 103014-24-0 103577-45-3 103922-27-6
103971-24-0 104340-41-2 104340-85-4 104658-07-3 104685-57-6
104987-90-8 105389-59-1 105950-65-0 105982-35-2 106747-09-5
107512-17-4 108026-58-0 108499-76-9 108662-50-6 109827-59-0
110405-59-9 110754-85-3 111371-25-6 111371-35-8 111476-81-4
111476-82-5 111476-83-6 111476-84-7 111476-85-8 111476-86-9
111476-87-0 111476-88-1 111476-89-2 111476-91-6 111476-92-7
111476-93-8 111476-94-9 111476-95-0 111476-96-1 111476-97-2
111476-98-3 111476-99-4 111477-01-1 111477-02-2 111477-03-3
111477-04-4 111604-52-5 111604-57-0 111858-83-4 112058-72-7
112058-73-8 112230-13-4 112645-53-1 112705-43-8 113209-69-1
113418-90-9 113703-12-1 113703-14-3 113703-20-1 113703-21-2

113703-22-3 113703-28-9 113712-97-3 113805-04-2 113855-38-2
113855-39-3 113855-40-6 113855-41-7 113855-42-8 113915-02-9
113942-61-3 114560-55-3 114878-71-6 115046-03-2 115366-78-4
115366-80-8 116091-77-1 116940-41-1 117038-05-8 117046-87-4
117347-86-1 117426-13-8 117934-10-8 117977-41-0 120009-37-2
120393-57-9 120699-85-6 120699-91-4 120894-71-5 121050-40-6
121242-23-7 121591-86-4 122307-32-8 122508-81-0 123215-59-8
123215-83-8 123451-58-1 123823-95-0 123907-70-0 123987-02-0
124736-45-4 124899-76-9 125214-42-8 126026-46-8 128429-74-3
128935-96-6 128936-05-0 130049-59-1 130368-60-4 130368-62-6
130368-66-0 133903-90-9 134017-66-6 134462-81-0 135430-38-5
135461-65-3 135863-25-1 137105-02-3 137247-56-4 137810-46-9
139644-93-2 139767-99-0 142062-72-4 150064-18-9 150460-06-3
153284-85-6 174398-06-2 174398-07-3 174398-08-4 174398-09-5
174398-10-8 174398-12-0 174398-13-1 174398-15-3 174398-20-0
187589-30-6 240118-16-5 240118-17-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

IT 366-18-7, 2,2'-Dipyridyl 400-98-6, 4-Trifluoromethyl-2-nitroaniline
446-33-3, 3-Fluoro-6-nitrotoluene 452-71-1, 4-Fluoro-2-methylaniline
455-14-1, 4-Trifluoromethylaniline 496-72-0, 3,4-Diaminotoluene
570-24-1, 2-Methyl-6-nitroaniline 583-39-1, 2-Mercaptobenzimidazole
616-86-4, 4-Ethoxy-2-nitroaniline 1603-41-4, 2-Amino-5-methylpyridine
1635-61-6, 3-Chloro-6-nitroaniline 1635-84-3, 2,4-Dimethyl-6-nitroaniline 1639-31-2, 3,4,5-Trimethylaniline 1824-81-3,
2-Amino-6-methylpyridine 3171-45-7, 4,5-Dimethyl-1,2-phenylenediamine
5327-33-3, 2-Acetamido-6-methylpyridine 5344-90-1, 2-Aminobenzyl alcohol
7595-31-5, 3,4-Dimethoxy-6-nitroaniline 23019-47-8 23612-57-9
27492-84-8, Methyl 4-amino-2-methoxybenzoate 37052-78-1,
2-Mercapto-5-methoxybenzimidazole 39785-37-0, 4-Methoxy-3,5-dimethylaniline 59338-85-1 61713-46-0 71675-52-0 71693-08-8
88301-76-2 88301-77-3 88301-78-4 88301-79-5 88301-81-9,
2-Chloromethylaniline hydrochloride 92333-53-4 92807-01-7
106746-59-2, 2-Chloromethyl-4-methoxyaniline hydrochloride 106746-62-7
106746-64-9 106746-67-2 106746-71-8 106746-73-0 106746-83-2
106746-85-4 106746-87-6 106746-89-8 106746-91-2 106746-92-3
106746-99-0 106771-59-9, 2-Chloromethyl-N,N-dimethylaniline
118267-31-5 174397-87-6 174397-89-8 175276-96-7 240118-15-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

IT 3287-79-4P, 5,6-Dimethyl-2-mercaptobenzimidazole 4093-29-2P, Methyl 4-acetamido-2-methoxybenzoate 25369-78-2P 25617-34-9P 27231-33-0P
55489-15-1P 59338-84-0P 73590-92-8P 74004-74-3P,
2-Mercapto-5,6-dimethoxybenzimidazole 86604-73-1P 86847-79-2P
106746-72-9P 106746-74-1P 106746-75-2P 106746-81-0P 106746-82-1P
106747-02-8P 106747-03-9P 106747-04-0P 106747-46-0P 106771-57-7P
118267-40-6P 118267-41-7P 174397-86-5P 174397-90-1P 174397-91-2P
174398-21-1P 174398-22-2P 240118-07-4P 240118-08-5P 240118-09-6P
240118-11-0P **240118-12-1P** **240118-13-2P** 240118-14-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of benzimidazolylsulfinylmethylarylamines as (H+/K+) ATPase inhibitors useful as antiviral agents)

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Adelstein; US 4772619 1988 CAPLUS
(2) Altamirano, A; Virology 1994, V199, P151 CAPLUS
(3) Anon; GB 2134523 1984 CAPLUS

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(6) Anon; EP 0167943 1986 CAPLUS
(7) Anon; EP 0178438 1986 CAPLUS
(8) Anon; EP 0194458 1986 CAPLUS
(9) Anon; EP 167943 1986 CAPLUS
(10) Anon; EP 178438 1986 CAPLUS
(11) Anon; EP 194458 1986 CAPLUS
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(14) Anon; EP 234690 1987 CAPLUS
(15) Anon; JP 230560 1989
(16) Anon; EP 335646 1989 CAPLUS
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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.85	369.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-5.54

FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004

Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4
DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

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  conducting SmartSELECT searches.

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> S 174398-05-1/RN

L17   1 174398-05-1/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

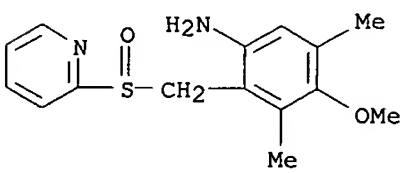
=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L17 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 5.92 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN   **174398-05-1** REGISTRY
CN   Benzenamine, 4-methoxy-3,5-dimethyl-2-[(2-pyridinylsulfinyl)methyl]- (9CI)
     (CA INDEX NAME)
FS   3D CONCORD
MF   C15 H18 N2 O2 S
SR   CA
LC   STN Files: CA, CAPLUS, USPATFULL



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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               2 REFERENCES IN FILE CA (1907 TO DATE)
               2 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF  FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     2.19     371.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -5.54

FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 21 Jan 2004  VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004  (20040120/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

     FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004
L1             STRUCTURE UPLOADED
L2           0 S L1 EXA SAM
L3           0 S L1 FAM SAM
L4          50 S L1 SSS SAM

     FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
L5          10 S L4

     FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004
L6        4073 S L1 SSS FULL
L7        3719 S HIV OR RETROVIRAL OR RETROVIRUS
L8        2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV
```

```
     FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004
L9         70667 S HIV OR RETROVIRAL OR RETROVIRUS
L10        31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV
L11          636 S L6
L12            9 S L11 AND L9

     FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004
L13            1 S 188839-16-9/RN
                 SET NOTICE 1 DISPLAY
                 SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004

     FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004
L14            1 S 457949-18-7/RN
                 SET NOTICE 1 DISPLAY
                 SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004
L15            5 S L11 AND L10
L16            2 S L15 NOT L12

     FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004
L17            1 S 174398-05-1/RN
                 SET NOTICE 1 DISPLAY
                 SET NOTICE LOGIN DISPLAY
                 SET NOTICE 1 DISPLAY
                 SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004

=> d l16 2 all

L16  ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1970:111444  CAPLUS
DN   72:111444
ED   Entered STN:  12 May 1984
TI   Antiviral and neuroleptic .alpha.-carbolines
PA   Glaxo Laboratories Ltd.
SO   Fr. Demande, 52 pp.
     CODEN: FRXXBL
DT   Patent
LA   French
IC   A61K; C07D
CC   28 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1
     PATENT NO.       KIND  DATE          APPLICATION NO.  DATE
     ---------------  ----  --------      ---------------  --------
PI   FR 2003999             19691114
     DE 1913119                           DE
     GB 1268772                           GB
     ZA 6901818             19690000      ZA
PRAI GB                     19680315
GI   For diagram(s), see printed CA Issue.
AB   The 2-substiuted .alpha.-carbolines (I) in which X is other than a halogen
     atom or an acyloxy group are prepd. by reaction of a salt (II) or a compd.
     (III) with a reactive nucleophile.  Thus, 2 g 1-methoxy-.alpha.-
     carbolinium methyl sulfate (IV) heated in a sealed tube at 110.degree.
     with 35 ml aq. NH4OH (d. 0.88) 4 hr gave 0.27 g unidentified compd. and
     further eluted with C6H6 contg. 50% AcOEt gave 38% 2-amino-.alpha.-
     carboline, m. 202-3.degree..  Similarly was obtained 2-hydrazino-.alpha.-
```

carboline, m. 185-7.degree.. Analogous treatment of IV provided I (R = H) (X and m.p. given): NHMe, 156-7.degree.; CN, 289-91.degree.; OMe, 167-9.degree.; SPh, 222-3.degree.; OCH2CH2NEt2, 117-19.degree.; HNCH2CH2NEt2, 102-3.degree.; SCH2CH2CH2Me, 179.0-8095.degree.; SCH2Ph, 182.5-3.0.degree.; SCH2CH2NEt2, 137.9.degree.; HN-(CH2)3Me,154-6.degree.; CH2CO2Et, 208-10.degree.; CH2CO2Et, 200-2.degree.; morpholino, 263-5.degree.; OH, 295.degree. (decompn.). Treatment of 0.9 g 1-methoxy-9-methyl-.alpha.-carbolinium methyl sulfate (V) i n 5 ml H2O with 0.5 g KCN in 2 ml H2O yielded I (R = Me, X = C N), m. 152-63.degree.. V in H2O stirred 2 hr with 40% aq. NaOH and the filtered soln. neutralized with 2N HCl yielded 34% I (R = Me, X = OH), m. 266-8.degree.. Dry PhMe (50 ml) contg. 3 g 1-ethoxy-.alpha.-carbolinium tetrafluoroborate, and 3.75 g. H2NCH2-CHMeOH refluxed 5 hr gave 0.32 g I (R = H, X = NHC h2CH-MeOH), m. 185-7.degree. (AcOEt). Similarly was obtained I (R = H, X = NH(CH2)3OH), m. 163-6.degree.. AcCH2CO2Et (4 ml) and 1-methoxy-.alpha.-isocarboline (from 1 g V) heated 2.5 hr on a steam bath and the cooled product treated with H2O gave 18.5 % I(R = H, X = CH2CO2Et), m. 200-2.degree.. Similarly were prepd. I(R = H, X = CH2COMe), m. 205-7.degree.; I[R = H, X = CH-(CN)2], m. 296-7.degree., and I (R = H, X = OMe), m. 166-9.degree., in 24, 12, and 23% yields. HO(CH2)5NH2 (30 ml) and 12 g 2-chloro-9-methyl-.alpha.-carboline heated in a sealed tube 16 hr at 200.degree. and the product partitioned between C6H6 and 2N aq. Na2CO3, the C6H6 ext. shaken with excess 2N HCl and filtered gave the HCl salt of I[R = Me, X = NH(CH2)5OH], m. 200-2.degree.. A mixt. of 10 g o-H2NC6H4NH2 and 25 g 2,6-Br2C5H3N heated 8 hr at 140.degree. and the product partitioned between CHCl3 and aq. Na2CO3, the C6H6 ext. shaken with excess 2N HCl and filtered gave the HCl salt of I [R = Me, X = NH(CH2)5OH], m. 200-2.degree.. A mixt. of 10 g o-H2NC6H4NH2 and 25 g 2,6-Br2C5H3N heated 8 hr at 140.degree. and the product partitioned between CHCl3 and aq. Na2CO3, the CHCl3 layer evapd. and the residue taken up on 500 g silica gel, eluted with C6H6 contg. increasing amts. of EtOAc gave 21 g unchanged 2,6-Br2C5H3N and 2.2 g 2-(o-amino anilino)-6-bromopyridine (VI), m. 141-2.degree. (iso-PrOH). VI (2.2 g) in 20 ml EtOH and 30 ml 5N HCl treated at 0.degree. with 1.03 g NaNO2 in 12 ml H2O gave 2.27 g 1-(6-bromopyrid-2-yl)benzo-triazole (VII), m. 115-16.degree. (EtOH). Benzotriazole (1 g) and 2 g 2,6-Br2C5H3N heated 5 min at 210.degree. with evolution of HBr and the cooled gum extd. with petroleum ether yielded 0.55 g VII. VII (3.5 g) and 20 g polyphosphoric acid heated 6 hr at 130.degree. and the coo led mixt. poured into H2O, filtered and the dried ppt. crystd. from C6 h6 gave 0.95 g I(R = H, X = Br) (VIII), m. 290.degree.. Benzotriazole (17.8 g) and 22.2 g 2,6-Cl2C5H3N heated 2 hr at 215.degree. (N atm.) and the cooled product extd. with 800 ml hot C6H12 gave 16 g 1-(6-chloropyrid-2-yl)benzotriazole (IX), m 130-1.degree.. Polyphosphoric acid (400 g) stirred at 180.degree. with addn. of 75 g IX and the mixt. kept 30 min at 160.degree., poured into 1 l. H2O and the dried ppt. crystd. in BuOAc gave 13.8 g I (R = H, X = Cl) (X) m. 271-3.degree.. X (5.06 g) in 120 ml MeO-CH2CH2OMe stirred with 0.72 g NaH 2.25hr and the pale yellow soln. kept 2.5 hr at 20.degree. with 4.26 g MeI gave 3.8 g I(R = Me, X = Cl)(XI), m. 126-8.degree.. The 2-halo-substituted compds. VIII, X, and XI heated with the nucl eophilic reagent under the specified conditions of time and temp. in a sea led tube (if necessary) gave the following I(R = H) (X and m.p. given): O(CH2)3Me, 178-9.degree.; O(CH2)2OH, 172-4.degree.; O(CH2)3OH, 178-9.degree.; O(CH2)2O(CH2)2OH, 147-9.degree.; [O(CH2)2]3OH, 100-1.degree.; NH2, 198-9.degree.; NH(CH2)3Me, 154-6.degree.; NH(CH2)7Me, 135-6.degree.; NEt2, -; morpholino, 263-5.degree.; 4-methylpyridazin-1-yl, 295-9.degree.; NHPh, 216-17.degree.; NH(CH2)2-OH, 180-3.degree.; NH(CH2)3OH, 167-9.degree.; NH(CH2)5OH, 137-8.degree.; NH(CH2)6OH, 155-7.degree.; NHCH2CH(OH)Me, 186-7.degree.; NH-(CH2)3OMe, 103-4.degree.; and also I (R = Me) (X and m.p. given): NHMe, 243-6.degree.; NH(CH2)3Me, 166-8.degree.; NH(CH2)5OH, 192-4.degree.; NHCH2CH2NEt2, 211-15.degree.. POCl3 (5.2 ml) stirred 30 min with 6.2 g 4-chloro-.alpha.-carboline 1-oxide in 60 ml HCONMe2 and the

mixt. heated 45 min on a steam bath, kept 18 hr at 20.degree. and poured into 500 ml H2O, neutralized with Na2CO3 and the ppt. crystd. from 100 ml MeOCH2CH2OH; the cryst. product (4.78 g) digested 1 hr in 60 ml EtOH and 60 ml 2N NaOH on a steam bath and dild. with H2O gave 4.38 g 2,4-dichloro-.alpha.-carboline (XII), m. 305-7.degree. (MeOCH2CH2OH). XII (0.5 g) and 7 ml BuNH2 heated in a sealed tube 19 hr at 200.degree. and the cooled mixt. freed from solvent, the dried residue triturated with dil . aq. Na2CO3 and the product recrystd. gave 0.48 g 2,4-di(butyl-amino)-.alpha.-carboline, m. 163-5.degree.. X (2.02 g) and 0.66 g NaH stirred 15 min in 40 ml MeCH(OMe)2 and the mixt. refluxed 8 hr with 5.3 g Me2N(CH2)3Cl in 30 ml C6H6, the residue on evapn. partitioned between C6H6 and H2O and the C6H6 layer evapd., the yellow gum (2.5 g) taken up in 10 ml EtOH and acidified with alc. HBr gave 2.2 g I[R = Me2N(CH2)3, X = Cl], HBr salt m. 215-18.degree. (alc.). Conversion of X by the above proce-dures gave I(R = H, X = SCH2CH2Me), m. 197-8.degree. (iso-PrOH) and I (R = Pr, X = Cl) (XIII), m. 77-8.degree. (iso-PrOH). XIII (1.09 g) and 6 ml BuO(CH2)3NH2 heated 16 hr at 200.degree. in a sealed tube gave I[R = Pr, X = NH(CH2)3OH], m. 89-91.degree. (Et2O) and I[R = Pr, X = NH(CH2)3OCHMe2], HBr salt m. 111-12.degree. (EtOAc). XII (0.5 g), 7 ml HCONMe2, and 0.5 ml POCl3 heated 1 hr on a steam bath and mixt. poured into 25 ml H2O gave 0.504 g solid. The solid (0.25 g) extd. by 30 ml 2:1 C6H12-C6H6 gave 2,4-dichloro-9-formyl-.alpha.-carboline, m. 150.0-60.5.degree.. PhNHMe (345 ml), 1.2 kg 2,6,3-Cl2(O2N)C5H2N, and 320 g NaHCO3 refluxed 2 hr in 10 l. EtOH and the hot filtered soln. cooled gave 1.142 kg 6-chloro-2-(N-methylanilino)-3-nitropyri-dine (XIV), m. 75-7.degree.. XIV (0.73 g) in 10 ml 10% aq. AcOH kept 30 min at 80.degree. with 3 g powd. Fe, the mixt. basified with aq. Na2CO3, and extd. with C6H6 gave 0.3 6 g 3-amino-6-chloro-2-(N-methylanilino)pyridine (XV), m. 94-7.degree.. XV (1.17 g) in 94 ml H2O and 12 ml H2SO4 treated dropwise at 5.degree. with 0.37 g NaNO2 in 10 ml H2O, the mixt. treated in 15 min with 4 g powd. Cu with heating to 45.degree., and extd. with EtOAc gave XI. Con-version of XI yielded I[R = Me, X = HO(CH2)3O], m. 74-6.degree.; I[R = Me, X = H2N(CH2)6NH](2HBr salt m. 251-3.degree.); I(R = Me, X = PhNH), m. 132-3.degree. (iso-PrOH). XI (5 g) shaken 18 hr with 10 ml concd. HNO3 (d. 1.42) and the mixt. poured into H2O yielded 58% 2-chloro-6-nitro-.alpha.-carboline (XVI), m. >410.degree.. Conversion of XVI yielded 29% 2-butylamino-6-nitro-.alpha.-car-boline m. 189-90.degree. (CHCl3); 32% 2-[2-(diethylamino)ethylamino]-6-nitro-.alpha.-carboline, m. 170-5.degree.; and 62% 9-benzyl-2-chloro-6-nitro-.alpha.-carboline, m. 220.degree. (EtOAc), further transformed to 63%. 9-benzyl-2-butylamino-6-nitro-.alpha.-carboline, m. 131-2.degree.. XI (3.5 g) in 40 ml CCl4 and 10 ml CHCl3 stirred 1 hr with 1.71 g Cl in CCl4 and treated with 30 ml 2N NaOH yielded 18% 2,6-dichloro-9-methyl-.alpha.-carboline (XVII), m. 188-90.degree. (ligroine). XVII (350 mg) and 2.5 ml BuNH2 heated 16 hr at 200.degree. in a sealed tube and the product partitioned between EtOAc and H2O, the EtOAc layer evapd. and the oil treated with alc. HCl and Et2O gave 0.4 g 2-butylamino-6-chloro-1-methyl-.alpha.-carboline-HCl, m. 194-6.degree. (alc.). XI was similarly converted to 6-chloro-2-(5-hydroxy-pentylamino)-9-methyl-.alpha.-carboline-HCl, m. 213.5-15.5.degree. (alc.). XVI reduced with NaH in dry glyme and treated with MeI gave 2-chloro-9-methyl-6-nitro-.alpha.-carboline, m. 269-71.degree. (BuOAc), converted to 2-butylamino-9-methyl-6-nitro-.alpha.-carboline, m. 90.degree. [(iso-Pr)2O]. [R = Me2N(CH2)3, X = Cl] HBr salt heated with BuNH2 at 210.degree. and the product treated with alc. HBr gave I[R = Me2N(CH2)3, X = BuNH2].2HBr, m. 213-16.degree.. I(R = H, X = MeNH), HCl salt (0.47 g) in 30 ml H2O basified with 4 ml 2N NaOH and extd. with EtOAc, the product taken up in 30 ml EtOH and refluxed 19 hr with 0.52 g morpholine and 0.67 ml 36% formol, the oily product taken up in 30 ml alc. and treated with the same amts. of morpholine and formol, refluxed 24 hr and the product extd. with Et2O yielded 38% I(R = N-mor-pholinomethyl, X = MeNH), m. 220.degree.. Hydrogenation of 250 mg 2-anilino-6-chloro-3-nitropyridine, m. 102-4.degree., in 25 ml EtOAc in the presence of 90 mg

10% Pd-C gave 238 mg 3-amino-2- anilino-6-chloropyridine, diazotized to give 50 mg 5-chloro-3-phenyltriazolo[4,5-b]pyridine, heated at 200.degree. with 0.3 g polyphosphoric acid to yield 3 mg X. Ac2O (40 ml) contg. 4 g .alpha.-carboline 1-oxide refluxed 30 min gave I(R = Ac, X = AcO), m. 155-7.degree., refluxed with aq NaOH and acidified with HCl to give 2-hydroxy-.alpha.-carboline, m. 294.degree. (decompn.), acetylated to 2-ace-toxy-.alpha.-carboline, m. 210.degree.. XII (2.4 g) in 100 ml MeOCH2CH2-OMe stirred 2 hr at 20.degree. with 0.338 g NaH and the soln. stirred 2 hr with 0.69 ml MeI, evapd. and the residue dild. with H2O gave 2.48 g 2,4-dichloro-9-methyl-.alpha.-carboline, m. 178-9.degree. (EtOAc). XI heated with BuNH2 at 200.degree. and the HCl salt crystd. from EtOH g ave I(R = Me, X = BuNH) HCl salt monoethanolate, dried 8 hr at 60 .degree./0.1 mm to yield the nonsolvated salt, m. 166-8.degree.. NaHCO3 (480 mg), 554 mg p-MeC6H4NH2 and 1 g 2,6-dichloro-3-nitropyridine refluxed 1 hr in 15 ml EtOH yielded 800 mg 6-chloro-3-nitro-2-(p-toluidino)pyridine, m. 116-19.degree. (iso-PrOH), converted by stirring with NaH in glyme and refluxing the soln. with MeI to give 400 mg 6-chloro- 2-(N-methyl-p-toluidino)-3-nitropyridine, m. 113-15.degree., reduced with powd. Fe in boiling AcOH to the corresponding 3-amino-6-chloro-2-(N-methyl-p-toluidino)pyridine (XVIII), m. 90-1.degree.. XVIII (750 mg) diazotized in 8 ml concd. H2SO4 and 8 ml H2O at 6.degree. with 230 mg NaNO2 in 4 ml H2O, stirred 1.5 hr with gradual addn. of 600 mg pptd. Cu and extd. with CHCl3 gave 500 mg 2-chloro-6,9-dimethyl-.alpha.-carboline, m. 132-4.degree. [(Me2CH)2O], converted to the correspond-ing 2-butylamino-6,9-dimethyl-.alpha.-carboline, m. 227-9.degree. (5:1 iso-PrOH-MeOCH2CH2OH). BuNH2 (7.5 ml) and 2 g 2-chloro-6-(N-methylanilino)-5-nitropyridine refluxed 30 min gave 2-(butylamino)-6-(N-methylanilino)-5-nitropyridine, m. 93-9.degree. (alc.), reduced catalytically over prereduced PtO2 and acidified to give 3-amino-6-butylamino-2-(N-methylanilino)pyridine-2-HBr, m. 170-92.degree. (decompn.). The base diazotized, heated with Cu powder at 30.degree. and the product analyzed chromatographically showed the presence of I(R = Me, X = BuNH). The compds. present a pronounced antiviral activity against **herpes** simplex, adenovirus SV 17, influenza A2, parainfluenza I, rhinovirus type I, rhinovirus type V and virus Coxsackie A 21, and show a surprising lack of toxicity on oral or subcutaneous administration. I(R = Me2N(CH2)3, X = Cl, shows neuroleptic activity.

ST antiviral neuroleptic carbolines; neuroleptic antiviral carbolines; carbolines antiviral neuroleptic

IT Virucides
(pyridoindole derivs.)

IT 6604-76-8P 25208-09-7P 25433-25-4P 26066-77-3P 26148-33-4P
26148-34-5P **26148-35-6P** 26148-36-7P 26148-37-8P
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26942-46-1P 26942-49-4P 27183-68-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

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=> FIL REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    3.73     375.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -0.69      -6.23

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=> S 26148-35-6/RN

L18           1 26148-35-6/RN

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=> D L18 SQIDE 1-

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L18  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   26148-35-6  REGISTRY
CN   9H-Pyrido[2,3-b]indole, 2-(benzylthio)- (8CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C18 H14 N2 S
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, TOXCENTER
         (*File contains numerically searchable property data)
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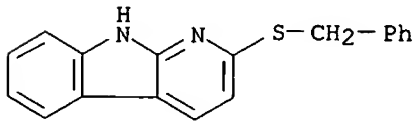

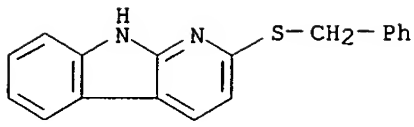

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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=> file caplus

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FULL ESTIMATED COST	3.87	379.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-6.23

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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> e antiviral

E1	6	ANTIVIR/BI
E2	1	ANTIVIRA/BI
E3	41240 -->	ANTIVIRAL/BI
E4	1	ANTIVIRALE/BI
E5	2	ANTIVIRALEN/BI
E6	103	ANTIVIRALLY/BI
E7	847	ANTIVIRALS/BI
E8	1	ANTIVIREMIC/BI

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E9          111     ANTIVIRIAL/BI
E10           2     ANTIVIRIALS/BI
E11           1     ANTIVIRICALLY/BI
E12           1     ANTIVIRIL/BI

=> s e3-e9
         41240 ANTIVIRAL/BI
             1 ANTIVIRALE/BI
             2 ANTIVIRALEN/BI
           103 ANTIVIRALLY/BI
           847 ANTIVIRALS/BI
             1 ANTIVIREMIC/BI
           111 ANTIVIRIAL/BI
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               BI OR ANTIVIRALS/BI OR ANTIVIREMIC/BI OR ANTIVIRIAL/BI)

=> s l19 and l11
L20          21 L19 AND L11

=> s l20 not l12
L21          15 L20 NOT L12

=> s l21 not l16
L22          13 L21 NOT L16

=> d l22 1-13

L22  ANSWER 1 OF 13  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2004:2860  CAPLUS
TI   Preparation of 8-(biaryl)quinolines as PDE4 inhibitors
IN   Deschenes, Denis; Dube, Daniel; Dube, Laurence; Gallant, Michel; Girard,
     Yves; Lacombe, Patrick; MacDonald, Dwight
PA   Merck Frosst Canada & Co., Can.
SO   PCT Int. Appl., 122 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.         KIND  DATE          APPLICATION NO.  DATE
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PI   WO 2004000814      A1    20031231      WO 2003-CA957    20030623
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ,
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             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
             NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
             GW, ML, MR, NE, SN, TD, TG
PRAI US 2002-391364P    P     20020625
     US 2002-428313P    P     20021122
RE.CNT  5     THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22  ANSWER 2 OF 13  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:980837  CAPLUS
DN   140:42459
TI   Preparation of dimethylcyclobutane amino acid derivatives as prenylation
     inhibitors
```

IN Brown, Bradley B.; Rehder, Kenneth S.; Strachan, Jon-Paul; Eaves, Jeron H.; Lowden, Christopher T.
PA PPD Discovery, Inc., USA
SO U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 219,851, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6664277	B1	20031216	US 2003-336186	20030103
PRAI US 2002-219851	B2	20020814		

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:913155 CAPLUS
DN 139:391329
TI Pyranone inhibitors of hepatitis C virus RNA-dependent RNA polymerase, and compositions and treatments using the same
IN Gonzalez, Javier; Borchardt, Allen John; Dragovich, Peter Scott; Jewell, Tanya Michelle; Linton, Maria Angelica; Zhou, Ru; Li, Hui; Tatlock, John Howard; Abreo, Melwyn A.; Prins, Thomas J.
PA Pfizer Inc., USA; et al.
SO PCT Int. Appl., 269 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003095441	A1	20031120	WO 2003-IB1905	20030507

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-379433P P 20020510
OS MARPAT 139:391329
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:757679 CAPLUS
DN 139:276825
TI Preparation of 8-arylquinoline PDE4 inhibitors
IN Gallant, Michel; Lacombe, Patrick; Dube, Daniel; Deschenes, Denis; MacDonald, Dwight; Dube, Laurence
PA Merck Frosst Canada & Co., Can.
SO PCT Int. Appl., 184 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 2003078397 A1 20030925 WO 2003-CA374 20030317
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 2002-365088P P 20020318
OS MARPAT 139:276825
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:504649 CAPLUS
DN 137:83638
TI Concomitant drugs of p38MAP kinase inhibitors and/or TNF-.alpha. prodn. inhibitors with other specified agents
IN Ohkawa, Shigenori; Naruo, Kenichi; Miwatashi, Seiji
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002051442	A1	20020704	WO 2001-JP11353	20011225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2002302458	A2	20021018	JP 2001-392778	20011225
EP 1354603	A1	20031022	EP 2001-271876	20011225
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRAI JP 2000-396220 A 20001226
JP 2001-27572 A 20010202
WO 2001-JP11353 W 20011225
OS MARPAT 137:83638
RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:256041 CAPLUS
DN 136:294826
TI Preparation of benzimidazolone **antiviral** agents
IN Yu, Kuo-Long; Civiello, Rita; Combrink, Keith; Gulgeze, Hatice Belgin; Pearce, Bradley C.; Wang, Xiangdong; Meanwell, Nicholas A.; Zhang, Yi
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 216 pp.
CODEN: PIXXD2
DT Patent

LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002026228	A1	20020404	WO 2001-US29493	20010927
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 6506738	B1	20030114	US 2001-952736	20010914
PRAI	US 2000-235804P	P	20000927		

OS MARPAT 136:294826
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:10451 CAPLUS
DN 136:85837
TI Preparation of benzodiazepines as inhibitors of HPV E1 helicase
IN Hurst, David Nigel; Jones, Philip Stephen; Parkes, Kevin Edward Burdon; Parratt, Martin John; Wilson, Francis Xavier
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000632	A1	20020103	WO 2001-EP6895	20010619
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1299364	A1	20030409	EP 2001-949420	20010619
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2002128262	A1	20020912	US 2001-892148	20010626
PRAI	GB 2000-15904	A	20000628		
	WO 2001-EP6895	W	20010619		

OS MARPAT 136:85837
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:31464 CAPLUS
DN 134:100762
TI Preparation of pyridine derivatives and medicinal use thereof
IN Iino, Yukio; Fujita, Kohichi; Kodaira, Ariko; Hatanaka, Toshihiro; Takehana, Kenji; Kobayashi, Tsuyoshi; Konishi, Atsushi; Yamamoto, Takashi
PA Ajinomoto Co., Inc., Japan
SO PCT Int. Appl., 86 pp.

CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002359	A1	20010111	WO 2000-JP4298	20000629
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1193255	A1	20020403	EP 2000-940879	20000629
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000012046	A	20020514	BR 2000-12046	20000629
	TW 519538	B	20030201	TW 2000-89113050	20000630
	US 2002133005	A1	20020919	US 2001-29871	20011231
PRAI	JP 1999-187959	A	19990701		
	JP 2000-71706	A	20000315		
	WO 2000-JP4298	W	20000629		

OS MARPAT 134:100762
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:772628 CAPLUS
DN 133:321879
TI Preparation of 5-pyridyl-1,3-azole compounds as antagonists of adenosine A3 receptor, process for producing the same and use thereof
IN Ohkawa, Shigenori; Kanzaki, Naoyuki; Miwatashi, Seiji
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 152 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064894	A1	20001102	WO 2000-JP2575	20000420
	W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1180518	A1	20020220	EP 2000-917375	20000420
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000009952	A	20020326	BR 2000-9952	20000420
	NZ 515215	A	20030725	NZ 2000-515215	20000420
	AU 765473	B2	20030918	AU 2000-38401	20000420
	JP 2001114779	A2	20010424	JP 2000-126289	20000421
	JP 3333774	B2	20021015		
	JP 2002363179	A2	20021218	JP 2002-164744	20000421
	NO 2001005156	A	20011218	NO 2001-5156	20011022

	ZA 2001008996	A	20030131	ZA 2001-8996	20011031
PRAI	JP 1999-116686	A	19990423		
	JP 1999-224650	A	19990806		
	WO 2000-JP2575	W	20000420		
	JP 2000-126289	A3	20000421		

OS MARPAT 133:321879
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:155490 CAPLUS
DN 124:202255
TI Preparation of sulfur-containing heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents
IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.
PA G. D. Searle and Co., USA
SO PCT Int. Appl., 212 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523950	A1	19951129	AU 1995-23950	19950501
	US 5945425	A	19990831	US 1996-737251	19961024
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	A2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		
	US 2000-605560	B1	20000627		

OS MARPAT 124:202255

L22 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:539204 CAPLUS
DN 119:139204
TI Preparation of 5-halothiazetoquinoline-3-carboxylic acid derivatives as antibacterial, antitumor, and anti-AIDS virus agents
IN Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Yoshida, Toshihiko; Yamamoto, Yoichi
PA Hokuriku Pharmaceutical, Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05059067	A2	19930309	JP 1991-252762	19910905
PRAI	JP 1991-252762		19910905		

OS MARPAT 119:139204

L22 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:32855 CAPLUS
DN 106:32855
TI 2,5-Bis(alkylsulfonyl)- and 2,5-bis(alkylthio)-substituted-pyridines
IN Wood, Steven G.
PA Dow Chemical Co., USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4616087	A	19861007	US 1982-380642	19820521
PRAI	US 1982-380642		19820521		

OS CASREACT 106:32855

L22 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:155211 CAPLUS
DN 98:155211
TI Sulfur-substituted phenoxypyridines having **antiviral** activity
IN Markley, Lowell D.; Tong, Yulan C.; Wood, Steven G.
PA Dow Chemical Co., USA
SO U.S., 22 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4371537	A	19830201	US 1981-292467	19810813
	ZA 8205762	A	19830629	ZA 1982-5762	19820809
	IL 66496	A1	19851129	IL 1982-66496	19820809
	CA 1180017	A1	19841225	CA 1982-409151	19820810
	EP 72529	A1	19830223	EP 1982-107263	19820811
	EP 72529	B1	19860129		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2103619	A1	19830223	GB 1982-23098	19820811
	GB 2103619	B2	19850227		
	AU 8287078	A1	19830512	AU 1982-87078	19820811
	AU 551683	B2	19860508		
	AT 17719	E	19860215	AT 1982-107263	19820811
	NO 8202751	A	19830214	NO 1982-2751	19820812
	NO 159851	B	19881107		
	NO 159851	C	19890215		
	DK 8203628	A	19830214	DK 1982-3628	19820812
	DK 157297	B	19891204		
	DK 157297	C	19900507		
	JP 58041868	A2	19830311	JP 1982-139277	19820812
	JP 04014107	B4	19920311		
	ES 514940	A1	19831016	ES 1982-514940	19820812
	ES 523661	A1	19850316	ES 1983-523661	19830628
	ES 523660	A1	19850401	ES 1983-523660	19830628
PRAI	US 1981-292467		19810813		
	EP 1982-107263		19820811		

OS CASREACT 98:155211

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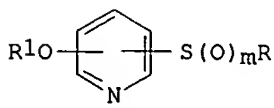
L22 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:155211 CAPLUS
DN 98:155211

ED Entered STN: 12 May 1984
TI Sulfur-substituted phenoxypyridines having **antiviral** activity
IN Markley, Lowell D.; Tong, Yulan C.; Wood, Steven G.
PA Dow Chemical Co., USA
SO U.S., 22 pp.
CODEN: USXXAM
DT Patent
LA English
IC A61K031-44; C07D021-263
NCL 424263000
CC 1-5 (Pharmacology)
Section cross-reference(s): 27
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4371537	A	19830201	US 1981-292467	19810813
	ZA 8205762	A	19830629	ZA 1982-5762	19820809
	IL 66496	A1	19851129	IL 1982-66496	19820809
	CA 1180017	A1	19841225	CA 1982-409151	19820810
	EP 72529	A1	19830223	EP 1982-107263	19820811
	EP 72529	B1	19860129		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2103619	A1	19830223	GB 1982-23098	19820811
	GB 2103619	B2	19850227		
	AU 8287078	A1	19830512	AU 1982-87078	19820811
	AU 551683	B2	19860508		
	AT 17719	E	19860215	AT 1982-107263	19820811
	NO 8202751	A	19830214	NO 1982-2751	19820812
	NO 159851	B	19881107		
	NO 159851	C	19890215		
	DK 8203628	A	19830214	DK 1982-3628	19820812
	DK 157297	B	19891204		
	DK 157297	C	19900507		
	JP 58041868	A2	19830311	JP 1982-139277	19820812
	JP 04014107	B4	19920311		
	ES 514940	A1	19831016	ES 1982-514940	19820812
	ES 523661	A1	19850316	ES 1983-523661	19830628
	ES 523660	A1	19850401	ES 1983-523660	19830628
PRAI	US 1981-292467		19810813		
	EP 1982-107263		19820811		

OS CASREACT 98:155211
GI



I

AB The title compds. I [R = C1-7 alkyl, C5 or C6 cycloalkyl, Ar(CH2)q (Ar = C6-10 aryl, q = 0-3), R1 = Ph or substituted Ph; m = 0, 1, or 2] preferably administered as pharmaceutical compns. (no data given) were prepd. by several methods and evaluated as **antiviral** agents. Thus, 2-(3,4-dichlorophenoxy)-5-(methylsulfonyl)pyridine [85331-30-2] prepd. by the reaction of 3,4-dichlorophenol [95-77-2] in DMSO in presence of Na tert-butoxide with 2,5-bis(methylsulfonyl)pyridine showed a broad spectrum **antiviral** activity at low conc. (25 .mu.g/mL).
ST phenoxythiopyridine prepn **antiviral**; virucide

phenoxythiopyridine; pyridine phenoxythio prepn **antiviral**

IT Virucides and Virustats
(phenoxythiopyridines)

IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**
85331-31-3P 85331-32-4P 85331-38-0P 85331-39-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation of)

IT 85331-36-8P 85331-37-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

IT 58819-71-9P 71506-85-9P 85330-62-7P 85330-65-0P 85330-68-3P
85330-69-4P 85330-71-8P 85330-74-1P **85330-77-4P**
85330-81-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

IT 85331-34-6P 85331-35-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with dichlorophenol)

IT 85330-72-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with hydroxyacetophenone)

IT **85330-78-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with hydroxybenzophenone)

IT 25935-30-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with sodium methanethiolate)

IT 85330-63-8P 85330-64-9P 85330-66-1P 85330-75-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with substituted phenols)

IT 25935-29-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)

IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P
85330-89-8P 85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P
85330-94-5P 85330-95-6P 85330-96-7P 85330-97-8P 85330-98-9P
85330-99-0P 85331-00-6P 85331-01-7P 85331-02-8P 85331-03-9P
85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P
85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P
85331-14-2P 85331-15-3P 85331-16-4P 85331-17-5P 85331-18-6P
85331-19-7P 85331-20-0P 85331-21-1P 85331-22-2P 85331-23-3P
85331-24-4P 85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P
85331-29-9P 85331-30-2P 85345-64-8P 85368-98-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and virucidal activity)

IT 62916-42-1P 85330-79-6P 85330-80-9P 85330-82-1P 85330-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 75-33-2
RL: BIOL (Biological study)
(reaction of with Me dichloropyridinecarboxylate)

IT 100-53-8 108-98-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Me dichloropyridinecarboxylate)
IT 95-95-4 533-31-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(ethylsulfonyl)pyridine)
IT 98-54-4 99-93-4 101-53-1 106-41-2 106-48-9 461-84-7 591-20-8
767-00-0 831-82-3 873-62-1 1073-72-9 1137-42-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(methylsulfonyl)pyridine)
IT 95-77-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloronitropyridine)
IT 140-89-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diazotized pyridine derivs.)
IT 4548-45-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichlorophenol)
IT 1569-69-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichloropyridinecarboxylic acid)
IT 75-08-1 111-31-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichlorpyridinecarboxylic acid)
IT 1532-24-7 1702-17-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with mercaptans)
IT 26452-80-2 85331-33-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methanethiol)
IT 74-93-1, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pyridinecarboxylates)

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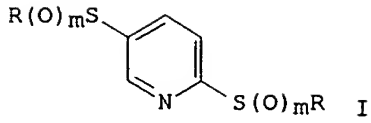
L22 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:32855 CAPLUS
DN 106:32855
ED Entered STN: 07 Feb 1987
TI 2,5-Bis(alkylsulfonyl)- and 2,5-bis(alkylthio)-substituted-pyridines
IN Wood, Steven G.
PA Dow Chemical Co., USA
SO U.S., 9 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D211-72
ICS C07D211-84
NCL 546294000
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4616087	A	19861007	US 1982-380642	19820521
PRAI US 1982-380642		19820521		

OS CASREACT 106:32855
GI



I

AB The title compds. I (R = C1-7 alkyl, cycloalkyl, Ar(CH2)q, Ar = (un)substituted Ph, naphthyl; q = 0-3; m = 0-2) useful as **antiviral** agents, were prepd. Thus, to 4-F3CSC6H4OH in THF was added Me3COK and 2,5-bis(methylsulfonyl)pyridine, prepd. in 3 steps from Me 3,6-dichloro-2-pyridinecarboxylate, to give 5-(methylsulfonyl)-2-[4-[(trifluoromethyl)thio]phenoxy]pyridine (II). II at 12.5 .mu.g/mL was active against rhinovirus type 1A.

ST pyridine alkylsulfonyl phenoxy prepn **antiviral**

IT Virucides and Virustats
(bis(alkylsulfonyl)- and bis(alkylthio)-substituted-pyridines)

IT 533-31-3, 3,4-(Methylenedioxy)phenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bis(ethylsulfonyl)pyridine)

IT 106-41-2, 4-Bromophenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bis(hexylsulfonyl)pyridine)

IT 461-84-7, 4-(Trifluoromethylthio)phenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bis(methylsulfonyl)pyridine)

IT 95-77-2, 3,4-Dichlorophenol 99-93-4, p-Hydroxyacetophenone 1137-42-4, p-Hydroxybenzophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with sulfonylpyridines)

IT 85330-64-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with (methylenedioxy)phenol)

IT 85330-63-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with (trifluoromethylthio)phenol)

IT 85330-69-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with bromophenol)

IT 85330-66-1P 85330-75-2P 85330-79-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with dichlorophenol)

IT 85330-72-9P 85330-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with hydroxyacetophenone)

IT **85330-78-5P** 85330-89-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with hydroxybenzophenone)

IT 85330-61-6P 85330-67-2P 85330-70-7P 85330-73-0P **85330-76-3P**
85331-32-4P 91164-62-4P 106025-37-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation of)

IT 85331-31-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and decarboxylation-oxidn. of)

IT 69212-36-8P 85330-62-7P 85330-65-0P 85330-68-3P 85330-71-8P
85330-74-1P **85330-77-4P** 85330-80-9P 85330-81-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

IT 98626-97-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 85330-84-3P 85330-85-4P 85330-86-5P 85330-87-6P 85330-88-7P
85330-90-1P 85330-91-2P 85330-92-3P 85330-93-4P 85330-96-7P
85330-97-8P 85330-98-9P 85330-99-0P 85331-02-8P 85331-03-9P
85331-04-0P 85331-05-1P 85331-06-2P 85331-07-3P 85331-08-4P
85331-09-5P 85331-10-8P 85331-11-9P 85331-12-0P 85331-13-1P
85331-14-2P 85331-15-3P 85331-16-4P 85331-17-5P 85331-18-6P
85331-25-5P 85331-26-6P 85331-27-7P 85331-28-8P 85345-64-8P
85368-98-5P 99902-97-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as virucide)
IT 74-93-1, reactions 75-33-2 111-31-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution by, of Me dichloropyridinecarboxylate)
IT 75-08-1 100-53-8, Benzyl mercaptan 108-98-5, Thiophenol, reactions
1569-69-3, Cyclohexyl mercaptan
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution by, of dichloropyridinecarboxylic acid)
IT 1702-17-6, 3,6-Dichloro-2-pyridinecarboxylic acid 88912-24-7,
5,6-Dichloro-2-pyridinecarboxylic acid
RL: PROC (Process)
(substitution of, with mercaptans)
IT 1532-24-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution with alkanethiol and hydrolysis of)

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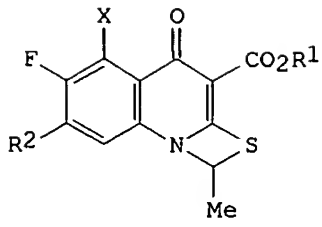
L22 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:539204 CAPLUS
DN 119:139204
ED Entered STN: 02 Oct 1993
TI Preparation of 5-halothiazetoquinoline-3-carboxylic acid derivatives as antibacterial, antitumor, and anti-AIDS virus agents
IN Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Yoshida, Toshihiko; Yamamoto, Yoichi
PA Hokuriku Pharmaceutical, Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07D513-04
ICS A61K031-47
CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05059067	A2	19930309	JP 1991-252762	19910905
PRAI	JP 1991-252762		19910905		

OS MARPAT 119:139204
GI



I

AB The title derivs. I [R1 = H, lower alkyl; R2 = halo, (un)substituted cyclic amino; X = halo) and their pharmaceutically acceptable salts, useful as bactericides, neoplasm inhibitors, and anti-AIDS virus agents (no data), are claimed. A DMF soln. of 16.0 g 5-chloro-6,7-difluoro-1,2-dihydro-4-hydroxy-2-thioxo-3-quinolinecabrolyic acid Et ester (prepn. given) was added dropwise to a mixt. of MeCHI2, K2CO3, and DMF at 90-100.degree. over 40 min to give 9.52 g I (R1 = Et, R2 = F, X = Cl).

ST thiazetoquinolinecarboxylate prepn antitumor antibacterial **antiviral**; AIDS virus inhibitor thiazetoquinolinecarboxylate prepn; neoplasm inhibitor thiazetoquinolinecarboxylic acid prepn; bactericide thiazetoquinolinecarboxylic acid prepn

IT Bactericides, Disinfectants, and Antiseptics
Neoplasm inhibitors
(thiazetoquinolinecarboxylic acid derivs.)

IT Acquired immune deficiency syndrome
(thiazetoquinolinecarboxylic acid derivs. for treatment of)

IT Virucides and Virustats
(thiazetoquinolinecarboxylic acid derivs., for human immunodeficiency virus-1)

IT Virus, animal
(human immunodeficiency, thiazetoquinolinecarboxylic acid derivs. as inhibitors for)

IT 64695-81-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

IT 149144-07-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of, (benzylthio)quinolinecarboxylic acid deriv. from)

IT 149144-09-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclocondensation of, with diiodoethane, thiazetoquinoline deriv. from)

IT 149144-04-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation and debromination of)

IT **149144-08-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, thioxoquinoline deriv. from)

IT 149636-28-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with Et chlorocarbonate, isothiocyanate from)

IT 149144-05-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with carbon disulfide, dithiocarbamate from)

IT 149144-06-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with di-Et malonate and methoxybenzyl chloride, [anilino(benzylthio)methylene]malonate deriv. from)
IT 149144-10-5P 149144-11-6P 149144-12-7P 149636-30-6P 149665-60-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antitumor and antibacterial and anti-AIDS virus agent)
IT 824-94-2, 4-Methoxybenzyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Ph isothiocyanate deriv. and di-Et malonate, [anilino(benzylthio)methylene]malonate deriv. from)
IT 105-53-3, Diethyl malonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Ph isothiocyanate deriv. and methoxybenzyl chloride, [anilino(benzylthio)methylene]malonate deriv. from)
IT 132883-43-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thiazetoquinoline deriv.)

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L22 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:155490 CAPLUS
DN 124:202255
ED Entered STN: 19 Mar 1996
TI Preparation of sulfur-containing heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents
IN Moormann, Alan E.; Becker, Daniel P.; Flynn, Daniel L.; Li, Hui; Villamil, Clara I.
PA G. D. Searle and Co., USA
SO PCT Int. Appl., 212 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D235-28
ICS A61K031-415; C07D401-12; A61K031-44; C07D233-84
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9529897	A1	19951109	WO 1995-US5021	19950501
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523950	A1	19951129	AU 1995-23950	19950501
	US 5945425	A	19990831	US 1996-737251	19961024
	US 2001047038	A1	20011129	US 2001-885221	20010620
PRAI	US 1994-235619	A2	19940429		
	WO 1995-US5021	W	19950501		
	US 1996-659098	B1	19960604		
	US 1999-377888	B1	19990819		
	US 2000-605560	B1	20000627		

OS MARPAT 124:202255
AB The title compds., which are (H+/K+) ATPase inhibitors, useful for the treatment of viral infections, are prepd. and formulations contg. them are

claimed. Thus, 2-[(1H-benzimidazol-2-yl)sulfinylmethyl]-N,N-dimethylbenzenamine, m.p. 107-109.degree., was prepd. and demonstrated a (H+/K+) ATPase IC50 of 0.7 .mu.M.

ST benzimidazolylsulfinylmethylmethylbenzenamine prepn ATPase inhibitor; **antiviral** agent prepn benzimidazolylsulfinylmethylmethylbenzenamin e; benzimidazolyl sulfinylmethylmethylbenzenamine

IT Ulcer inhibitors
Virucides and Virustats
(heterocyclic (H+/K+) ATPase inhibitors)

IT 9000-83-3, ATPase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(potassium-hydrogen-activated; prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 55546-06-0P 56713-45-2P 57235-18-4P 60524-97-2P 71670-48-9P
73590-36-0P 73590-58-6P 73590-61-1P 81527-04-0P 81864-40-6P
81864-65-5P 94452-40-1P 96733-60-7P 97288-52-3P 97963-93-4P
97966-85-3P 98412-35-2P 98412-41-0P 99153-80-7P 99153-89-6P
99499-40-8P 100924-68-3P 101387-98-8P 102127-07-1P 102127-11-7P
102625-70-7P 102625-79-6P 103014-24-0P 103577-45-3P 103922-27-6P
103971-24-0P 104340-33-2P 104340-34-3P 104340-35-4P 104340-37-6P
104340-38-7P 104340-41-2P 104340-86-5P 104524-67-6P 104524-68-7P
104658-07-3P 104685-57-6P 104987-90-8P 105389-48-8P 105950-65-0P
105982-35-2P 106746-58-1P 106746-60-5P 106746-61-6P 106746-63-8P
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111502-75-1P 111604-57-0P 111858-83-4P 112058-72-7P 112058-73-8P
112230-13-4P 112645-53-1P 112705-43-8P 113418-90-9P 113703-12-1P
113703-14-3P 113703-21-2P 113703-22-3P 113703-28-9P 113712-97-3P
113805-04-2P 113855-38-2P 113855-39-3P 113855-40-6P 113855-41-7P
113855-42-8P 113915-02-9P 113942-61-3P 114060-19-4P 114560-55-3P
115046-03-2P 115366-78-4P 115366-80-8P 116091-77-1P 116940-41-1P
117038-05-8P 117046-87-4P 117347-86-1P 117426-11-6P 117934-10-8P
117977-41-0P 118267-21-3P 118267-22-4P 118267-23-5P 118267-24-6P
118267-25-7P 118267-26-8P 118267-27-9P 118267-28-0P 118267-29-1P
118267-30-4P 118267-31-5P 118267-32-6P 118267-33-7P 118267-34-8P
118267-35-9P 118267-36-0P 118267-37-1P 118267-38-2P 118267-39-3P
118267-42-8P 118267-43-9P 118292-92-5P 118292-93-6P 118292-94-7P
118292-95-8P 118292-96-9P 118292-97-0P 118292-98-1P 118292-99-2P
120009-37-2P 120393-57-9P 120699-85-6P 120699-91-4P 120894-65-7P
121050-40-6P 121242-64-6P 121591-86-4P 122223-85-2P 122307-32-8P
122508-81-0P 123215-59-8P 123215-83-8P 123451-58-1P 123823-95-0P
123907-70-0P 123987-02-0P 124736-45-4P 124899-76-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 125214-42-8P 126026-46-8P 128429-74-3P 128935-96-6P 128936-05-0P
130049-59-1P 130368-60-4P 130368-62-6P 130368-66-0P 133903-90-9P
134017-66-6P 134462-81-0P 135430-38-5P 135461-65-3P 135863-25-1P
137105-02-3P 137247-56-4P 137810-46-9P 139644-93-2P 139767-99-0P
142062-72-4P 150064-18-9P 150460-06-3P 153284-85-6P 174397-92-3P
174397-93-4P 174397-94-5P 174397-95-6P 174397-96-7P 174397-97-8P
174397-98-9P 174397-99-0P 174398-00-6P 174398-01-7P 174398-02-8P
174398-03-9P 174398-04-0P **174398-05-1P** 174398-06-2P
174398-07-3P 174398-08-4P 174398-09-5P 174398-10-8P 174398-11-9P
174398-12-0P 174398-13-1P 174398-14-2P 174398-15-3P 174398-16-4P
174398-17-5P 174398-18-6P 174398-19-7P 174398-20-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 144114-21-6, Retropepsin
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 85-44-9, Phthalic anhydride 94-09-7, Ethyl 4-aminobenzoate 110-18-9
140-89-6, Potassium ethylxanthate 400-98-6, 4-(Trifluoromethyl)-2-nitroaniline 446-33-3, 3-Fluoro-6-nitrotoluene 455-14-1, 4-(Trifluoromethyl)aniline 583-39-1, 2-Mercaptobenzimidazole 1603-41-4, 2-Amino-5-methylpyridine 1635-61-6, 3-Chloro-6-nitroaniline 1635-84-3, 2,4-Dimethyl-6-nitroaniline 1639-31-2, 3,4,5-Trimethylaniline 1824-81-3, 2-Amino-6-methylpyridine 2127-03-9, 2,2'-Dipyridyl disulfide 3171-45-7, 4,5-Dimethyl-1,2-phenylenediamine 3287-79-4, 2-Mercapto-5,6-dimethylbenzimidazole 5327-33-3, 2-Acetamido-6-methylpyridine 5344-90-1, 2-Aminobenzyl alcohol 7595-31-5 25369-78-2 27231-33-0, 2-Mercapto-4-methylbenzimidazole 27231-36-3 27492-84-8, Methyl 4-amino-2-methoxybenzoate 30525-89-4, Paraformaldehyde 37052-78-1, 2-Mercapto-5-methoxybenzimidazole 39785-37-0, 4-Methoxy-3,5-dimethylaniline 55489-15-1 71675-52-0, 2-(Bromomethyl)-4-chloroaniline hydrobromide 71693-08-8, 2-(Bromomethyl)-5-chloroaniline hydrobromide 74004-74-3 86604-73-1 88301-76-2 88301-77-3 88301-78-4 88301-79-5 88301-81-9, 2-(Chloromethyl)aniline hydrochloride 90562-37-1, N-[2-(Chloromethyl)phenyl]acetamide 92333-53-4 92643-51-1 92807-01-7 106746-59-2, 2-(Chloromethyl)-4-methoxyaniline hydrochloride 106746-62-7 106746-64-9 106746-67-2 106746-71-8 106746-85-4 106746-87-6 106746-89-8 106746-91-2 106746-92-3 106746-99-0 106771-59-9, 2-(Chloromethyl)-N,N-dimethylaniline 174397-86-5 174397-87-6 174397-88-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as **antiviral** agents)

IT 4093-29-2P, Methyl 4-acetamido-2-methoxybenzoate 25617-34-9P
27841-33-4P 59338-85-1P, Methyl 4,5-diamino-2-methoxybenzoate
86847-79-2P 104524-65-4P 106746-72-9P 106746-73-0P 106746-74-1P
106746-75-2P 106746-81-0P 106746-82-1P 106746-83-2P 106747-02-8P
106747-03-9P 106747-04-0P 106747-46-0P 106771-57-7P 118267-40-6P
165685-25-6P 174397-89-8P 174397-90-1P 174397-91-2P 174398-21-1P
174398-22-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of sulfur-contg. heterocyclic (H+/K+) ATPase inhibitors as

antiviral agents)

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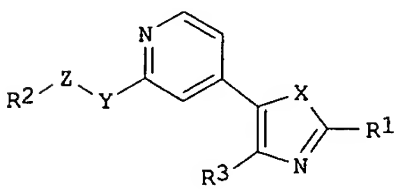
L22 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:772628 CAPLUS
DN 133:321879
ED Entered STN: 03 Nov 2000
TI Preparation of 5-pyridyl-1,3-azole compounds as antagonists of adenosine A3 receptor, process for producing the same and use thereof
IN Ohkawa, Shigenori; Kanzaki, Naoyuki; Miwatashi, Seiji
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 152 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07D417-04
ICS C07D417-14; A61K031-4439; A61P043-00; A61P029-00; A61P031-12; A61P003-10; A61P001-00; A61P009-00; A61P007-00
CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064894	A1	20001102	WO 2000-JP2575	20000420
	W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1180518	A1	20020220	EP 2000-917375	20000420
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000009952	A	20020326	BR 2000-9952	20000420
	NZ 515215	A	20030725	NZ 2000-515215	20000420
	AU 765473	B2	20030918	AU 2000-38401	20000420
	JP 2001114779	A2	20010424	JP 2000-126289	20000421
	JP 3333774	B2	20021015		
	JP 2002363179	A2	20021218	JP 2002-164744	20000421
	NO 2001005156	A	20011218	NO 2001-5156	20011022
	ZA 2001008996	A	20030131	ZA 2001-8996	20011031
PRAI	JP 1999-116686	A	19990423		
	JP 1999-224650	A	19990806		
	WO 2000-JP2575	W	20000420		
	JP 2000-126289	A3	20000421		

OS MARPAT 133:321879
GI



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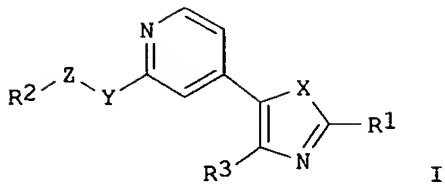

I

AB Optionally N-oxidized compds. represented by general formula (I) salts thereof [wherein R1 represents hydrogen, hydrocarbyl, a heterocycle, amino or acyl; R2 represents an arom. group; R3 represents hydrogen, pyridyl or arom. hydrocarbyl; X represents oxygen or optionally oxidized sulfur; Y represents a bond, oxygen, optionally oxidized sulfur or NR4 (wherein R4 represents hydrogen, hydrocarbyl, or acyl); and Z represents a bond or a divalent chain hydrocarbyl] are prepd. These compds. are usable as preventives or remedies for diseases in assocn. with adenosine A3 receptor because of having excellent adenosine A3 receptor antagonism thereof. Moreover, the compds. I or salts thereof exhibit excellent effects of inhibiting p38 MAP kinase and inhibiting TNF-.alpha. and, therefore, are also usable as preventives or remedies for diseases in assocn. with p38 MAP kinase or TNF-.alpha.. Above diseases include asthma, allergies, brain edema, cerebral vascular disorders, head injuries, inflammation, Addison's disease, autoimmune hemolytic anemia, Crohn's disease, psoriasis, rheumatism, spinal cord injury, multiple sclerosis, Alzheimer's disease, Parkinson's disease, amyotrophic lateral sclerosis, diabetes, arthritis, septemia, ulcerative colitis, chronic pneumonia, silicosis, lung sarcoidosis, pulmonary tuberculosis, cachexia, arteriosclerosis, Creutzfeldt-Jakob disease, virus infection, atopic dermatitis, systemic lupus erythematosus, AIDS encephalopathy, meningitis, angina pectoris, myocardial infarction, ischemic heart failure, hepatitis, transplant, dialysis hypotension, and frequent disseminated intravascular coagulation. Thus, bromination of 2-(2-benzoylamino-4-pyridyl)-1-(4-methoxyphenyl)ethanone with Br in AcOH at room temp. for 1 h followed by cyclocondensation of the bromination product with thiourea in the presence of Et3N in MeCN at 80.degree. for 5 h gave N-[4-[2-amino-4-(4-methoxyphenyl)-1,3-thiazol-5-yl]-2-pyridyl]benzamide (II). II showed IC50 of 0.020 .mu.M against p38 MAP kinase and 0.014 .mu.M for inhibiting the prodn. of TNF-.alpha. in THP-1 cells.

ST pyridylazole prepn antagonist adenosine A3 receptor; pyridylthiazole prepn TNF alpha inhibitor; p38 MAP kinase inhibitor pyridylthiazole

IT Adenosine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(A3; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
Prion diseases
(Creutzfeldt-Jakob; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Intestine, disease
(Crohn's; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Nervous system
(amyotrophic lateral sclerosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease

(angina pectoris; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Dermatitis
(atopic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
(cerebrovascular; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Pneumonia
(chronic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Blood coagulation
(disseminated intravascular, frequent; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
(edema; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease
(failure, ischemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Anemia (disease)
(hemolytic, autoimmune; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Brain, disease
(in assocn. with AIDS; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Hypotension
(in assocn. with dialysis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Heart, disease
(infarction; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Head
Spinal cord
(injury; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Addison's disease
Allergy inhibitors
Alzheimer's disease
Anti-inflammatory agents
Antiarteriosclerotics
Antiarthritics
Antiasthmatics
Antidiabetic agents
Antirheumatic agents
Antiviral agents
Cachexia
Hepatitis
Meningitis
Multiple sclerosis

Parkinson's disease
Psoriasis
Septicemia
Silicosis
Transplant and Transplantation
Tuberculosis
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Tumor necrosis factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lung, disease
(sarcoidosis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Lupus erythematosus
(systemic; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT Intestine, disease
(ulcerative colitis; prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-57-4P 303162-71-2P 303162-72-3P 303162-74-5P 303162-75-6P
303162-76-7P 303162-77-8P 303162-78-9P 303162-79-0P 303162-80-3P
303162-85-8P 303162-86-9P 303162-87-0P 303162-88-1P 303162-89-2P
303162-90-5P 303162-91-6P 303162-92-7P 303162-93-8P 303162-94-9P
303162-95-0P 303162-96-1P 303163-15-7P 303163-17-9P 303163-18-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 303162-58-5P 303162-59-6P 303162-60-9P 303162-61-0P 303162-62-1P
303162-64-3P 303162-66-5P 303162-67-6P 303162-68-7P 303162-69-8P
303162-70-1P 303162-73-4P 303162-81-4P 303162-82-5P 303162-83-6P
303162-84-7P 303162-97-2P 303162-98-3P 303162-99-4P 303163-00-0P
303163-01-1P 303163-02-2P 303163-03-3P 303163-04-4P 303163-05-5P
303163-06-6P 303163-07-7P 303163-08-8P 303163-09-9P 303163-10-2P
303163-11-3P 303163-12-4P 303163-13-5P 303163-14-6P 303163-16-8P
303163-19-1P 303163-20-4P 303163-21-5P 303163-22-6P 303163-23-7P
303163-24-8P 303163-25-9P 303163-26-0P 303163-27-1P 303163-28-2P
303163-29-3P 303163-30-6P 303163-31-7P 303163-32-8P 303163-33-9P
303163-34-0P 303163-35-1P 303163-36-2P 303163-37-3P 303163-38-4P
303163-39-5P 303163-40-8P 303163-41-9P 303163-42-0P
303163-43-1P 303163-44-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 165245-96-5, p38 MAP kinase
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 62-55-5, Thioacetamide 62-56-6, Thiourea, reactions 64-04-0, 2-Phenylethylamine 74-88-4, Methyl iodide, reactions 75-36-5, Acetyl chloride 75-55-8 98-88-4, Benzoyl chloride 100-07-2,

4-Methoxybenzoyl chloride 100-46-9, Benzylamine, reactions 100-51-6, Benzenemethanol, reactions 100-53-8, Phenylmethanethiol 103-67-3, N-Benzyl-N-methylamine 103-80-0, Phenylacetyl chloride 104-86-9, 4-Chlorobenzylamine 108-98-5, Thiophenol, reactions 109-74-0, Butyronitrile 110-59-8, Valeronitrile 140-75-0, 4-Fluorobenzylamine 499-06-9, 3,5-Dimethylbenzoic acid 589-08-2, N-Methyl-2-phenylethylamine 598-52-7, N-Methylthiourea 631-58-3, Thiopropionamide 645-45-4, 3-Phenylpropionyl chloride 772-70-3, 3-(4-Fluorophenyl)propionyl chloride 873-32-5, 2-Chlorobenzonitrile 1194-02-1, 4-Fluorobenzonitrile 1711-05-3, 3-Methoxybenzoyl chloride 1711-06-4, 3-Methylbenzoyl chloride 2243-83-6, 2-Naphthoyl chloride 2393-23-9, 4-Methoxybenzylamine 2627-86-3, (S)-1-Phenylethylamine 3886-69-9, (R)-1-Phenylethylamine 4152-90-3, 3-Chlorobenzylamine 4926-28-7, 2-Bromo-4-methylpyridine 5071-96-5, 3-Methoxybenzylamine 5271-67-0, 2-Thiophenecarbonyl chloride 6850-57-3, 2-Methoxybenzylamine 15893-42-2, 3-(4-Methoxyphenyl)propionyl chloride 18496-54-3, 4-Phenylbutyryl chloride 20260-53-1, Nicotinoyl chloride hydrochloride 20371-41-9, 5-Phenylvaleryl chloride 21382-98-9, 4-Methylthiobenzonitrile 27757-85-3, 2-Thienylmethylamine 90101-20-5, 2-(tert-Butoxycarbonylamino)-4-methylpyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

IT 461-87-0P, 2-Fluoro-4-methylpyridine 6613-44-1P, 3,5-Dimethylbenzoyl chloride 15717-17-6P, 2-Chlorothiobenzamide 16536-93-9P, Thiobutyramide 16536-94-0P, Thiovaleramide 21384-43-0P 22179-72-2P, 4-Fluorothiobenzamide 53550-91-7P, 4-(Methylthio)thiobenzamide
102336-06-1P 224040-60-2P 224040-71-5P 303162-27-8P 303162-28-9P
303162-29-0P 303162-30-3P 303162-31-4P 303162-32-5P 303162-33-6P
303162-34-7P 303162-35-8P 303162-36-9P 303162-37-0P 303162-38-1P
303162-39-2P 303162-40-5P 303162-41-6P 303162-42-7P 303162-43-8P
303162-44-9P 303162-45-0P 303162-46-1P 303162-47-2P 303162-48-3P
303162-49-4P 303162-50-7P 303162-52-9P 303162-54-1P 303162-55-2P
303162-56-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyridylazole compds. as antagonists of adenosine A3 receptor and inhibitors of TNF-.alpha. and p38 MAP kinase for therapeutics)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(2) Merck & Co Inc; CN 1203590 A CAPLUS
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(4) Merck & Co Inc; US 5717100 A CAPLUS
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(7) Merck & Co Inc; SK 9800435 A
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L22 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:31464 CAPLUS
DN 134:100762
ED Entered STN: 12 Jan 2001
TI Preparation of pyridine derivatives and medicinal use thereof
IN Iino, Yukio; Fujita, Kohichi; Kodaira, Ariko; Hatanaka, Toshihiro; Takehana, Kenji; Kobayashi, Tsuyoshi; Konishi, Atsushi; Yamamoto, Takashi
PA Ajinomoto Co., Inc., Japan
SO PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC C07D211-58; C07D213-75; C07D213-76; C07D237-20; C07D237-22; C07D239-42; C07D239-48; C07D277-44; A61K031-44; A61K031-445; A61K031-50; A61K031-505; A61P029-00
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002359	A1	20010111	WO 2000-JP4298	20000629
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1193255	A1	20020403	EP 2000-940879	20000629
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	TW 519538	B	20030201	TW 2000-89113050	20000630
	US 2002133005	A1	20020919	US 2001-29871	20011231
PRAI	JP 1999-187959	A	19990701		
	JP 2000-71706	A	20000315		
	WO 2000-JP4298	W	20000629		

OS MARPAT 134:100762
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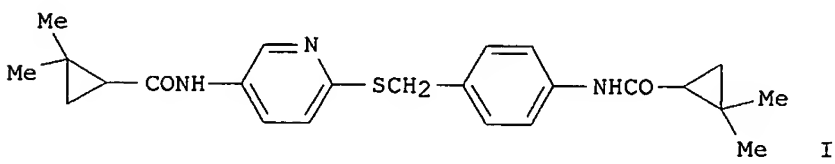

I

AB Heterocyclic compds. represented by the following general formula R1-CO-N(R2)-A-X-B-N(R3)-Y-(CH2)n-R4 [R1 = (un)substituted or cycloalkenyl; R2, R3 = H, alkyl; R4 = (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, or heterocyclyl having .gtoreq.1 heteroatom(s); A = (un)substituted heterocyclic ring; B = (un)substituted arom. or heterocyclic ring; n = 0-6; Y = a bond between atoms, CO, CO2, CONR5, C(S)NR5, SO, SO2 (wherein R5 = H, alkyl); X = a bond between atoms, O,

OCHR7, CHR8O, O2C, CO2, OC(S), C(S)O, S, SO, SO2, SCHR9, CHR10S, SC(O), C(O)S, SC(S), C(S)S, SO2 NR11, NR12SO2, NR13, etc.; R7 - R10 = H, alkyl; R11 - R13 = H, alkyl, acyl] or pharmacol. acceptable salts thereof are prepd. These compds. have inhibitory effects on AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor, etc. and are usable as drugs such as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics. Thus, 2-mercapto-5-nitropyridine was treated with NaH in DMF and then alkylated by 1-bromomethyl-4-nitrobenzene at room temp. for 1.5 h to give 2-(4-nitrobenzylthio)-5-nitropyridine which was reduced by Zn/AcOH in THF at room temp. for 16 h to 2-(4-aminobenzylthio)-5-aminopyridine and then acylated by 2,2-dimethylcyclopropanecarbonyl chloride in the presence of Et3N in CH2Cl2 at room temp. for 17 h to give 2-(4-(2,2-dimethylcyclopropanecarbonylamino)benzylthio)-5-(2,2-dimethylcyclopropanecarbonylamino)pyridine (I). I in vitro inhibited NF-kappa B activity with IC50 of 0.015 .mu.g/mL in an assay measuring .beta.-galactosidase activity expressed in HUVEC cells and driven by NF-kappa B-binding sequence-fused SV40 T antigen min. promoter.

ST pyridine prepn antiinflammatory; antirheumatic pyridine prepn; **antiviral** immunosuppressant pyridine prepn; cancer metastasis inhibitor pyridine prepn; antiarteriosclerotics pyridine prepn

IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(AP-1 (activator protein 1); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(NF-.kappa. B (nuclear factor .kappa. B); prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cell adhesion
(factor, inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Cytokines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inflammatory; prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT Antitumor agents
(metastasis; prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT Anti-inflammatory agents
Antiarteriosclerotics
Antirheumatic agents
Antiviral agents
Immunosuppressants
(prepn. of pyridine derivs. as antiinflammatory, antirheumatic, **antiviral** agents, immunosuppressants, cancer metastasis inhibitors, and antiarteriosclerotics)

IT 318967-19-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 318967-14-5P 318967-15-6P 318967-16-7P 318967-17-8P 318967-18-9P
318967-20-3P 318967-21-4P 318967-22-5P 318967-23-6P 318967-24-7P
318967-25-8P 318967-26-9P **318967-27-0P** 318967-28-1P
318967-29-2P 318967-30-5P 318967-31-6P 318967-32-7P 318967-33-8P
318967-34-9P 318967-35-0P 318967-36-1P 318967-37-2P 318967-38-3P
318967-39-4P 318967-40-7P 318967-41-8P 318967-42-9P 318967-43-0P
318967-44-1P 318967-45-2P 318967-46-3P 318967-47-4P 318967-48-5P
318967-49-6P 318967-50-9P 318967-51-0P 318967-52-1P 318967-53-2P
318967-54-3P 318967-55-4P 318967-56-5P 318967-57-6P 318967-58-7P
318967-59-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 81669-70-7, Metalloprotease
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 88-75-5, 2-Nitrophenol 98-09-9, Benzenesulfonyl chloride 98-88-4, Benzoyl chloride 100-02-7, 4-Nitrophenol, reactions 100-11-8, 4-Nitrobenzyl bromide 103-63-9, 2-Bromoethylbenzene 103-71-9, Phenyl isocyanate, reactions 103-72-0, Phenyl isothiocyanate 103-80-0, Phenylacetyl chloride 104-03-0, 4-Nitrophenylacetic acid 108-24-7, Acetic anhydride 122-04-3, 4-Nitrobenzoyl chloride 123-30-8, 4-Hydroxyaniline 554-84-7, 3-Nitrophenol 636-98-6, 1-Iodo-4-nitrobenzene 637-59-2, 3-Phenylpropyl bromide 661-69-8, Hexamethylditin 932-67-2, 3-Cyclohexenecarbonyl chloride 1821-12-1, 4-Phenylbutanoic acid 1849-36-1, 4-Nitrobenzenethiol 2127-09-5, 2-Mercapto-5-nitropyridine 2581-34-2, 3-Methyl-4-nitrophenol 2719-27-9, Cyclohexanecarbonyl chloride 3073-77-6, 2-Amino-5-nitropyrimidine 3958-57-4, 3-Nitrobenzyl bromide 3958-60-9, 2-Nitrobenzyl bromide 4487-59-6, 2-Bromo-5-nitropyridine 4548-45-2, 2-Chloro-5-nitropyridine 4693-91-8, 4-Methoxyphenylacetyl chloride 5339-26-4, 2-(4-Nitrophenyl)ethyl bromide 5365-15-1, 2,2-Dichlorocyclopropanecarbonyl chloride 5418-51-9, 2-Hydroxy-5-nitropyridine 5469-69-2, 3-Amino-6-chloropyridazine 7169-97-3, 2-Acetamido-5-bromopyridine 10313-60-7, 3,4-Dimethoxyphenylacetyl chloride 14221-01-3, Tetrakis(triphenylphosphine)palladium 23056-33-9, 2-Chloro-4-methyl-5-nitropyridine 24424-99-5, Di-tert-butyl dicarbonate 25026-34-0, 4-Chlorophenylacetyl chloride 33332-29-5 39053-78-6, 3,4,5-Trimethoxyphenylacetyl chloride 50541-93-0, 4-Amino-1-benzylpiperidine 50675-57-5, 2,2-Dimethylcyclopropanecarbonyl chloride 54840-15-2, 4-(tert-Butoxycarbonylamino)phenol 55972-71-9, p-Phenylenediamine hydrochloride 60733-34-8, 2-Methylcyclopropanecarbonyl chloride 69097-20-7, Tris(trimethylsiloxy)ethylene 89312-77-6 90403-98-8, 2-Methylcyclohexanecarbonyl chloride 103554-20-7 193204-58-9 318967-66-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)

IT 4982-09-6P 13534-97-9P, 5-Amino-2-bromopyridine 24253-19-8P
29958-19-8P 32605-02-0P 34295-27-7P 99844-01-6P 109899-69-6P
116735-74-1P 318967-60-1P 318967-61-2P 318967-62-3P 318967-63-4P
318967-64-5P 318967-65-6P 318967-67-8P 318967-68-9P 318967-69-0P
318967-70-3P 318967-71-4P 318967-72-5P 318967-73-6P 318967-74-7P
318967-75-8P 318967-76-9P **318967-77-0P 318967-78-1P**
318967-79-2P 318967-80-5P 318967-81-6P 318967-82-7P 318967-83-8P
318967-84-9P 318967-85-0P 319459-36-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyridine derivs. as inhibitors of AP-1 activity, NF-kappa B activity, inflammatory cytokine prodn., matrix metalloprotease prodn., expression of inflammatory cell adhesion factor)
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Ajinomoto Co Inc; WO 200015603 A1 2000
(2) Boehringer Ingelheim Pharmaceuticals Inc; JP 2000502702 A
(3) Boehringer Ingelheim Pharmaceuticals Inc; US 6057451 A CAPLUS
(4) Boehringer Ingelheim Pharmaceuticals Inc; WO 9724343 A1 1997 CAPLUS
(5) Smithkline Beecham Corp; JP 2000500464 A
(6) Smithkline Beecham Corp; JP 2000500464 A
(7) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
(8) Smithkline Beecham Corp; EP 866700 A1 CAPLUS
(9) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS
(10) Smithkline Beecham Corp; WO 9717958 A1 1997 CAPLUS

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L22 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:10451 CAPLUS
DN 136:85837
ED Entered STN: 04 Jan 2002
TI Preparation of benzodiazepines as inhibitors of HPV E1 helicase
IN Hurst, David Nigel; Jones, Philip Stephen; Parkes, Kevin Edward Burdon; Parratt, Martin John; Wilson, Francis Xavier
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D243-14
ICS C07D401-06; C07D403-06; C07D471-04; C07D401-12; C07D417-12; C07D413-12; C07D403-12; C07D487-04; A61K031-5513; A61K031-5517; A61K031-5517; C07D471-04; C07D243-00; C07D209-00; C07D487-04; C07D243-00; C07D235-00
CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002000632	A1	20020103	WO 2001-EP6895	20010619
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1299364	A1	20030409	EP 2001-949420	20010619

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

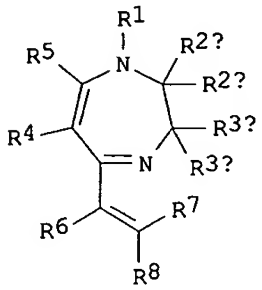
US 2002128262 A1 20020912 US 2001-892148 20010626

PRAI GB 2000-15904 A 20000628

WO 2001-EP6895 W 20010619

OS MARPAT 136:85837

GI



I

AB Novel benzodiazepin derivs. of general formula (I; R1 = H, lower alkyl, lower alkenyl, lower alkynyl, aryl lower alkyl, lower alkyl carbonyl, aryl carbonyl, lower alkyl aminocarbonyl, aryl aminocarbonyl, lower alkoxycarbonyl, aryloxycarbonyl; R2a, R2b = H or lower alkyl or R2a and R2b together are oxo, R1 and R2a or R2b together with the nitrogen and the carbon atom to which they are attached form an optionally substituted heterocycle; R3a, R3b = = H or lower alkyl; R4 and R5 together with the two carbon atoms to which they are attached form an optionally substituted aryl or an optionally substituted heterocycle; R6, R7 = H or lower alkyl; and R8 = optionally substituted aryl or heterocyclyl) or pharmaceutically acceptable salts thereof are prepd. The novel compds. are inhibitors of the human papilloma virus (HPV) E1 helicase enzyme which is involved in the viral replication and can therefore be used as therapeutic agents for HPV mediated diseases such as visible genital warts (sexually transmitted disease) and benign external warts. Thus, a mixt. of 1.475 g (5 mmol) of (E)-3-(3,4-dichlorophenyl)-1-(2-fluorophenyl)propenone and 1.1 g (5.45 mmol) of N-[2-(isopropylamino)ethyl]pivalamide was refluxed in 10 mL of pyridine for 6 h, followed by evapn. of the solvent and silica gel chromatog. to give (26 mg E)-3-(3,4-dichlorophenyl)-1-(2-(N-(2-pivaloylaminoethyl)isopropylamino)phenyl)-2-propen-1-one as a yellow gum. The latter compd. was added a soln. of 50 mg (0.26 mmol) of 4-toluenesulfonic acid in 5 mL of acetonitrile and refluxed for 30 s, followed by evapn. of the solvent, and the residue was treated with 5 mL of methanol and 50 mg (0.5 mmol) of triethylamine and refluxed for 1 min to give, after work-up and treatment with HCl/EtOAc, (E)-5-(3,4-dichlorostyryl)-2,3-dihydro-1-isopropyl-1H-1,4-benzodiazepine dihydrochloride (II). II and (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride showed IC50 of .mu.g/mL against of 1.6 and 2 .mu.M, resp., against helicase.

ST benzodiazepine prepn inhibitor HPV E1 helicase; styryldihydrobenzodiazepine prepn human papilloma virus E1 helicase; visible genital wart treatment styryldihydrobenzodiazepine prepn; benign external wart treatment styryldihydrobenzodiazepine prepn

IT Human papillomavirus
(E1; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT Enzymes, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(RNA helicase; prepn. of benzodiazepines as inhibitors of HPV E1

helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT **Antiviral** agents
Wart
(prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 386214-96-6P, (E)-5-(3,4-Difluorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-12-9P, (E)-5-(2-Benzylthio-5-nitrostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-36-7P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-nitro-1H-1,4-benzodiazepine hydrochloride 386215-67-4P, (E)-2,3-Dihydro-1-methyl-5-[5-nitro-2-(3-phenylpropylthio)styryl]-1H-1,4-benzodiazepine 386215-85-6P 386216-22-4P, (E)-5-(3,4-Dichlorostyryl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one 386216-24-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-benzo-1,4-diazepine dihydrochloride 386216-30-4P 386216-48-4P 386216-58-6P 386216-68-8P 386216-74-6P 386216-75-7P 386216-86-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 204130-58-5P, 2-(N-Benzyl-N-methylamino)-5-nitrobenzaldehyde 386214-97-7P, [1-Methyl-1,2,3,4-tetrahydrobenzo[e][1,4]diazepin-5-ylidenemethyl]phosphonic acid diethyl ester 386214-98-8P, [2-(2-Fluorophenyl)-2-oxoethyl]phosphonic acid diethyl ester 386215-19-6P, N-Methoxy-N-methyl-2-phenethylbenzamide 386215-25-4P 386215-41-4P 386215-46-9P 386215-48-1P 386215-51-6P 386215-89-0P 386215-99-2P 386216-04-2P 386216-06-4P 386216-09-7P 386216-16-6P, (E)-N-[[N-[2-[3-(3,4-Dichlorophenyl)acryloyl]phenyl]-N-methylcarbamoyl]methyl]pivalamide 386216-17-7P 386216-18-8P 386216-19-9P, N-[[N-(2-Acetylphenyl)-N-methylcarbamoyl]methyl]pivalamide 386216-25-7P, (E)-3-(3,4-Dichlorophenyl)-1-(2-fluorophenyl)propenone 386216-31-5P, (3-Acetyl-4-fluorophenyl)carbamic acid tert-butyl ester 386216-39-3P, N-[2-(Isopropylamino)ethyl]pivalamide 386216-40-6P, (E)-3-(3,4-Dichlorophenyl)-1-(2-(N-(2-pivaloylaminoethyl)isopropylamino)phenyl)-2-propen-1-one 386216-59-7P, Ethyl (E)-2-[5-(3,4-dichlorostyryl)-2,3-dihydro-1,4-benzodiazepin-1-yl]acetate 386216-64-4P 386216-69-9P, [2-(4-Formylbenzoylamino)ethyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 386216-27-9P 386216-70-2P 386216-91-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 386214-99-9P, (E)-5-(4-Butoxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-00-5P, (E)-2,3-Dihydro-1-methyl-5-(3-phenoxystyryl)-1H-1,4-benzodiazepine dihydrochloride 386215-01-6P, (E)-5-(3-Bromo-4-methoxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-02-7P, (E)-5-[3-Fluoro-4-(trifluoromethyl)styryl]-2,3-dihydro-1-methyl-1H-benzo[e][1,4]diazepine dihydrochloride 386215-03-8P 386215-04-9P 386215-05-0P **386215-06-1P** 386215-07-2P 386215-08-3P 386215-09-4P 386215-10-7P 386215-11-8P, (E)-5-(2-Fluorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-13-0P, (E)-5-[2-[(2-Chloro-5-

thiazolyl)methoxy]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine 386215-14-1P, (E)-5-[2-(tert-Butylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine 386215-15-2P, (E)-5-(2-Hexyloxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine 386215-16-3P, (E)-2,3-Dihydro-1-methyl-5-[5-nitro-2-(3-pyridyloxy)styryl]-1H-1,4-benzodiazepine 386215-17-4P, (E)-5-(5-Bromo-2-isopropoxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine 386215-18-5P, (E)-2,3-Dihydro-1-methyl-5-[2-(2-phenylethyl)styryl]-1H-1,4-benzodiazepine 386215-20-9P, (E)-2,3-Dihydro-1-methyl-5-(2-methylthiostyryl)-1H-1,4-benzodiazepine 386215-21-0P 386215-22-1P, (E,E)-2,3-Dihydro-1-methyl-5-(2-styrylstyryl)-1H-1,4-benzodiazepine 386215-23-2P 386215-24-3P, (E,E)-2,3-Dihydro-1-methyl-5-[2-(styrylthio)styryl]-1H-1,4-benzodiazepine 386215-26-5P 386215-27-6P, (E)-5-[2-(Cyclohexylmethylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine 386215-28-7P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-pyrido[2,3-e][1,4]diazepine hydrochloride 386215-29-8P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-pyrido[3,4-e][1,4]diazepine 386215-30-1P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-pyrido[3,2-e][1,4]diazepine 386215-31-2P 386215-32-3P, (E)-5-(3,4-Dichlorostyryl)-8-(trifluoromethyl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine hydrochloride 386215-33-4P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-8-methoxy-1-methyl-1H-1,4-benzodiazepine hydrochloride 386215-34-5P 386215-35-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-7-nitro-1H-1,4-benzodiazepine 386215-37-8P, (E)-5-(3,4-Dichlorostyryl)-9-(trifluoromethyl)-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386215-38-9P, (E)-5-(3,4-Dichlorostyryl)-8-(trifluoromethyl)-2,3-dihydro-1H-1,4-benzodiazepine hydrochloride 386215-39-0P 386215-40-3P, (E)-8-Bromo-5-(3,4-dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-42-5P 386215-43-6P, (E)-5-(2-Benzylthio-5-nitrostyryl)-8-bromo-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride **386215-44-7P** 386215-45-8P, (E)-9-Chloro-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386215-47-0P 386215-49-2P, (E)-5-(2-Benzylthio-5-nitrostyryl)-7-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-50-5P, (E)-8-Chloro-5-(3,4-dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-52-7P 386215-53-8P, (E)-5-(3-Allyloxystyryl)-8-chloro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-54-9P, (E)-5-(3-Benzyloxystyryl)-8-chloro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-55-0P, (E)-5-(2-Benzylthiostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-56-1P 386215-57-2P, (E)-5-[2-(4-Chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-58-3P, (E)-5-[2-(3,4-Dichlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-59-4P, 5-[3-Chloro-2-(4-chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-60-7P, (E)-2,3-Dihydro-1-methyl-5-(5-nitro-2-phenoxystyryl)-1H-1,4-benzodiazepine dihydrochloride 386215-61-8P, (E)-2,3-Dihydro-1-methyl-5-[2-(4-methylbenzylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-62-9P, (E)-2,3-Dihydro-5-[2-(4-methoxybenzylthio)styryl]-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-63-0P, (E)-5-[2-(4-Chlorophenoxy)-5-nitrostyryl]-3,4-dihydro-1-methyl-1H-1,4-benzodiazepine hydrochloride 386215-64-1P, (E)-5-[2-(4-tert-Butylbenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-65-2P, (E)-5-[2-[3-(Trifluoromethyl)benzylthio]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-66-3P, (E)-5-[4-Bromo-2-(4-chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-68-5P, (E)-2,3-Dihydro-1-methyl-5-(2-pentylthiostyryl)-1H-1,4-benzodiazepine 386215-69-6P, (E)-5-[2-Chloro-6-(4-chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine hydrochloride 386215-70-9P, 2-[2-(2,3-Dihydro-1-methyl-1H-1,4-benzodiazepin-5-yl)vinyl]-N-methyl-4-nitroaniline dihydrochloride

386215-71-0P 386215-72-1P, (E)-5-[2-(4-Chlorophenoxy)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-73-2P, (E)-2,3-Dihydro-1-methyl-5-[2-(2-naphthyloxy)-5-nitrostyryl]-1H-1,4-benzodiazepine dihydrochloride 386215-74-3P, (E)-2,3-Dihydro-1-methyl-5-[2-(1-naphthyloxy)-5-nitrostyryl]-1H-1,4-benzodiazepine dihydrochloride 386215-75-4P, (E)-2,3-Dihydro-1-methyl-5-(2-p-tolylthiostyryl)-1H-1,4-benzodiazepine dihydrochloride 386215-76-5P, (E)-2,3-Dihydro-5-[2-(4-methoxyphenylthio)styryl]-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-77-6P, (E)-2,3-Dihydro-1-methyl-5-[2-(2-naphthylthio)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-78-7P, (E)-2,3-Dihydro-1-methyl-5-[2-[(2-naphthyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-79-8P, (E)-5-[2-[4-(Trifluoromethyl)benzyloxy]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-80-1P, (E)-2,3-Dihydro-1-methyl-5-[2-(4-nitrobenzyloxy)styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-81-2P, (E)-5-[2-(3,4-Difluorobenzyloxy)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-82-3P, (E)-5-(2-Benzyloxystyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-83-4P, (E)-5-[2-(4-Chlorobenzyloxy)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-84-5P 386215-86-7P 386215-87-8P 386215-88-9P, (E)-2,3-Dihydro-1-methyl-5-[3-[(2-pyridyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-90-3P, (E)-2,3-Dihydro-1-methyl-5-[3-[(3-pyridyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-91-4P, (E)-2,3-Dihydro-1-methyl-5-[3-[(4-pyridyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-92-5P, (E)-2,3-Dihydro-1-methyl-5-[3-[(5-methyl-3-isoxazolyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-93-6P, (E)-5-[3-[(1-Benzyl-1H-imidazol-2-yl)methoxy]styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-94-7P, (E)-5-[2,3-Dihydro-3-(4-methoxybenzyloxy)styryl]-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386215-95-8P 386215-96-9P, (E)-2,3-Dihydro-1-methyl-5-[3-[(3,5-dimethyl-1-pyrazolyl)methoxy]styryl]-1H-1,4-benzodiazepine dihydrochloride 386215-97-0P 386215-98-1P, (E)-5-[2-(4-Chlorophenoxy)styryl]-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-00-8P, (E)-5-[3-Chloro-2-(3,4-dichlorobenzylthio)styryl]-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-01-9P, (E)-5-(2-Benzylthiostyryl)-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-02-0P, (E)-5-(2-Benzylthio-5-nitrostyryl)-8-fluoro-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-03-1P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-8-(3-methoxyphenyl)-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-05-3P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-phenyl-1H-1,4-benzodiazepine dihydrochloride 386216-07-5P 386216-08-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-(3-thienyl)-1H-1,4-benzodiazepine dihydrochloride 386216-10-0P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-9-phenyl-1H-1,4-benzodiazepine hydrochloride 386216-11-1P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-9-(4-methoxyphenyl)-1H-1,4-benzodiazepine hydrochloride 386216-12-2P, (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1-methyl-8-(3-thienyl)-1H-1,4-benzodiazepine dihydrochloride 386216-13-3P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-vinyl-1H-1,4-benzodiazepine dihydrochloride 386216-14-4P, (E)-5-[2-(4-Chlorophenylthio)styryl]-8-(2-furyl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-15-5P, (E)-5-(3,4-Dichlorostyryl)-1,3-dihydro-1-methyl-2H-benzo-1,4-diazepin-2-one 386216-20-2P, (E)-1,3-Dihydro-5-styryl-2H-benzo-1,4-diazepin-2-one 386216-21-3P, (E)-5-(2,3-Dichlorostyryl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one 386216-23-5P, (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1H-1,4-benzodiazepine hydrochloride 386216-26-8P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-benzo-1,4-diazepine dihydrochloride 386216-29-1P 386216-32-6P, (E)-5-(3,4-Dichlorostyryl)-1-ethyl-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386216-33-7P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-

propyl-1H-1,4-benzodiazepine dihydrochloride 386216-34-8P, (E)-1-Benzyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386216-35-9P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine-1-ethanol dihydrochloride 386216-36-0P, (E)-5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386216-37-1P 386216-38-2P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-isopropyl-1H-1,4-benzodiazepine dihydrochloride 386216-41-7P, (E)-1-Acetyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine hydrochloride 386216-43-9P, (E)-1-Benzoyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine hydrochloride 386216-44-0P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-(4-nitrobenzyl)-1H-1,4-benzodiazepine dihydrochloride 386216-45-1P 386216-46-2P 386216-47-3P 386216-49-5P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-[(2-naphthyl)methyl]-1H-1,4-benzodiazepine dihydrochloride 386216-50-8P, (E)-4-[[5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepin-1-yl]methyl]benzoic acid dihydrochloride 386216-52-0P, (E)-3-[[5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepin-1-yl]methyl]benzoic acid hydrochloride 386216-54-2P, (E)-2-[[5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepin-1-yl]methyl]benzoic acid hydrochloride 386216-56-4P, (E)-4-[[5-[2-(4-Chlorophenylthio)styryl]-2,3-dihydro-1H-1,4-benzodiazepin-1-yl]methyl]benzoic acid hydrochloride 386216-57-5P, (E)-5-(3,4-Dichlorostyryl)-N-ethyl-2,3-dihydro-1H-1,4-benzodiazepine-1-carboxamide 386216-60-0P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-N-(2-methoxyethyl)-1H-1,4-benzodiazepine-1-acetamide dihydrochloride 386216-61-1P 386216-63-3P 386216-65-5P 386216-66-6P 386216-67-7P 386216-71-3P 386216-72-4P 386216-73-5P 386216-76-8P 386216-77-9P 386216-78-0P 386216-79-1P 386216-80-4P 386216-81-5P, 4-[2-(2,3-Dihydro-1-methyl-1H-1,4-benzodiazepin-5-yl)vinyl]benzamide hydrochloride 386216-82-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-8-ol hydrochloride 386216-83-7P 386216-85-9P 386216-87-1P, (E)-N-[5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-7-yl]methanesulfonamide 386216-88-2P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-8-(4-methoxyphenyl)-1-methyl-1H-1,4-benzodiazepine 386216-89-3P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-(2-thienyl)-1H-1,4-benzodiazepine hydrochloride 386216-90-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-8-amine hydrochloride 386216-93-9P 386216-94-0P 386216-95-1P 386216-97-3P, (E)-2,3-Dihydro-5-(4-methoxystyryl)-1-methyl-1H-1,4-benzodiazepine hydrochloride 386216-98-4P, (E)-2,3-Dihydro-1-methyl-5-(4-phenoxystyryl)-1H-1,4-benzodiazepine hydrochloride 386216-99-5P, (E)-2,3-Dihydro-1-methyl-5-styryl-1H-1,4-benzodiazepine dihydrochloride 386217-00-1P, (E)-5-(3,4-Dichlorostyryl)-1,3-dihydro-7,8-dimethoxy-2H-1,4-benzodiazepin-2-one 386217-01-2P, (E)-1-Acetyl-5-(3,4-dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine dihydrochloride 386217-02-3P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-1,4-benzodiazepine-1-ethanol hydrochloride 386217-03-4P 386217-04-5P, 5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-8-vinyl-1H-1,4-benzodiazepine dihydrochloride 386217-05-6P 386217-06-7P 386217-07-8P 386217-08-9P 386217-09-0P 386217-10-3P, (E)-5-[3-Chloro-2-(4-chlorobenzylthio)styryl]-2,3-dihydro-1-methyl-1H-1,4-benzodiazepine dihydrochloride 386217-11-4P 386224-42-6P, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1-methyl-1H-1,4-benzodiazepin-7-acetamide hydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

IT 67-36-7, 4-Phenoxybenzaldehyde 90-02-8, 2-Hydroxybenzaldehyde, reactions 93-97-0, Benzoic anhydride 98-80-6, Phenylboronic acid 100-11-8, 4-Nitrobenzyl bromide 100-52-7, Benzaldehyde, reactions 100-53-8,

Benzylmercaptan 103-67-3, N-Benzylmethylamine 105-36-2, Ethyl bromoacetate 106-48-9, 4-Chlorophenol 107-15-3, Ethylenediamine, reactions 109-81-9, N-Methylethylenediamine 109-85-3, 2-Methoxyethylamine 109-90-0, Ethyl isocyanate 110-72-5, N-Ethylethylenediamine 111-39-7, N-Propylethylenediamine 111-41-1, 2-(2-Aminoethylamino)ethanol 123-11-5, 4-Methoxybenzaldehyde, reactions 147-93-3, Thiosalicylic acid 445-29-4, 2-Fluorobenzoic acid 446-30-0, 4-Chloro-2-fluorobenzoic acid 446-52-6, 2-Fluorobenzaldehyde 450-95-3, 2-Fluoroacetophenone 543-24-8, N-Acetylglycine 551-93-9, 2'-Aminoacetophenone 586-98-1, 2-Pyridylmethanol 598-21-0, Bromoacetyl bromide 619-66-9, 4-Carboxybenzaldehyde 636-72-6, Thiophene-2-methanol 939-26-4, 2-Bromomethylnaphthalene 1126-81-4, 4-Acetamidothiophenol 1129-28-8, Methyl 3-(bromomethyl)benzoate 1571-08-0, Methyl 4-formylbenzoate 1583-58-0, 2,4-Difluorobenzoic acid 1859-75-2, 2'-(Methylamino)acetophenone 2393-23-9, 4-Methoxybenzylamine 2417-72-3, Methyl 4-(bromomethyl)benzoate 2417-73-4, Methyl 2-(bromomethyl)benzoate 2991-28-8, 2,5-Difluorobenzoic acid 2999-46-4, Ethyl isocyanoacetate 3006-96-0, 4-Hydroxymethylbenzoic acid 3095-95-2, Diethylphosphonoacetic acid 4152-09-4, N-Benzylethylenediamine 4392-24-9, Cinnamyl bromide 4890-85-1, 2-Phenethylbenzoic acid 5071-96-5, 3-Methoxybenzylamine 5720-07-0, 4-Methoxyphenylboronic acid 6165-68-0, Thiophene-2-boronic acid 6165-69-1, Thiophene-3-boronic acid 6258-66-8, 4-Chlorobenzylmercaptan 6287-38-3, 3,4-Dichlorobenzaldehyde 6334-18-5, 2,3-Dichlorobenzaldehyde 6361-21-3, 2-Chloro-5-nitrobenzaldehyde 6361-22-4, 2-Chloro-6-nitrobenzaldehyde 6850-57-3, 2-Methoxybenzylamine 7486-35-3, Vinyltributylstannane 10365-98-7, 3-Methoxyphenylboronic acid 19522-67-9, N-Isopropylethylenediamine 24424-99-5, Di-tert-butyl dicarbonate 32832-96-5, 2-Phenethylbenzaldehyde 34036-07-2, 3,4-Difluorobenzaldehyde 36480-40-7, 3,4-Dichlorobenzyl mercaptan 57260-73-8, N-(2-Aminoethyl)carbamic acid tert-butyl ester 67500-19-0, 1-(5-Amino-2-fluorophenyl)ethanone 85070-48-0, 3-Chloro-2-fluorobenzaldehyde 107572-07-6, 2-(4-Chlorophenylthio)benzaldehyde 112704-79-7, 2-Fluoro-4-bromobenzoic acid 118486-94-5, 2-(Tributylstannyl)furan 142265-69-8, 1-(2-Fluoro-4,5-dimethoxyphenyl)ethanone 161957-55-7, 2-Fluoro-3-chlorobenzoic acid 174013-29-7, 2-Fluoro-6-trifluoromethylacetophenone 175278-43-0, 2-Benzylthio-5-nitrobenzaldehyde 376646-64-9, 3-Formyl-4-(3-bromophenyl)pyridine 386216-28-0 386216-42-8, (E)-5-(3,4-Dichlorostyryl)-2,3-dihydro-1H-benzo-1,4-diazepine 386216-51-9 386216-53-1 386216-55-3 386216-92-8, 4-(3-Bromophenyl)-2-formylpyridine 386216-96-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of benzodiazepines as inhibitors of HPV E1 helicase and therapeutic agents for HPV mediated diseases such as visible genital warts and benign external warts)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

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TI Preparation of benzimidazolone **antiviral** agents

IN Yu, Kuo-Long; Civiello, Rita; Combrink, Keith; Gulgeze, Hatice Belgin; Pearce, Bradley C.; Wang, Xiangdong; Meanwell, Nicholas A.; Zhang, Yi
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 216 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-4184
ICS A61K031-443; A61K031-422; A61K031-427; A61K031-454; A61K031-501; A61K031-5377; C07D401-14; C07D403-06; C07D403-14; C07D413-14; C07D417-14
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
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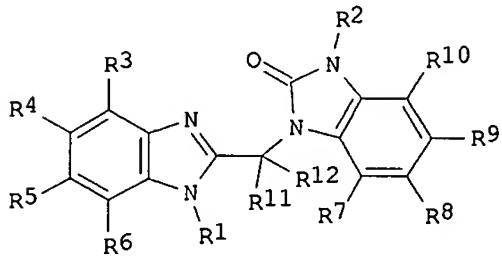
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002026228	A1	20020404	WO 2001-US29493	20010927
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 6506738	B1	20030114	US 2001-952736	20010914
PRAI US 2000-235804P	P	20000927		

OS MARPAT 136:294826
GI



I

AB The title compds. [I; R1 = (CRvRw)nX; Rv, Rw = H, (halo)alkyl, (halo)alkenyl; X = H, (un)substituted alkyl, alkenyl; n = 1-6; R2 = H, alkyl, Ph, etc.; R3, R6, R7, R10 = H; R5, R8, R9 = H, halo, CF3; R4 = H, halo, CN, etc.; R11, R12 = H], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a 4-step synthesis of I [R1 = CH2CH2CHMe2; R2 = C(:CH2)Me; R3-R12 = H], starting with 2-(chloromethyl)benzimidazole, was given. The title compds. I showed **antiviral** activity against RSV with EC50's between 50 .mu.M and 0.001 .mu.M.
ST benzimidazolone prepn **antiviral** respiratory syncytial virus RSV
IT **Antiviral** agents
(prepn. of benzimidazolone **antiviral** agents)
IT Respiratory syncytial virus
(treatment of RSV infection; prepn. of benzimidazolone **antiviral** agents)
IT 406940-52-1P 406940-54-3P 406940-55-4P 406940-56-5P 406940-57-6P
406940-63-4P 406940-76-9P 406941-33-1P 406941-36-4P 406941-69-3P

406941-70-6P 406941-71-7P 406941-78-4P 406941-83-1P 406941-84-2P
406941-87-5P 406941-89-7P 406941-92-2P 406941-93-3P 406942-22-1P
406942-26-5P 406942-39-0P 406942-55-0P 406942-56-1P 406942-59-4P
406942-60-7P 406942-63-0P 406942-68-5P 406942-72-1P 406942-82-3P
406942-84-5P 406942-86-7P 406942-87-8P 406943-03-1P 406943-05-3P
406943-11-1P 406943-18-8P 406943-20-2P 406943-22-4P 406943-25-7P
406943-29-1P 406943-53-1P 406943-55-3P 406943-56-4P 406943-68-8P
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406943-97-3P 406944-07-8P 406944-12-5P 406944-22-7P 406944-23-8P
406944-36-3P 406944-45-4P 406944-48-7P 406944-59-0P 406944-76-1P
406945-21-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of benzimidazolone **antiviral** agents)

IT 406940-53-2P 406940-58-7P 406940-59-8P 406940-60-1P 406940-61-2P
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406940-69-0P 406940-71-4P 406940-73-6P 406940-75-8P 406940-77-0P
406940-78-1P 406940-79-2P 406940-81-6P 406940-82-7P 406940-83-8P
406940-84-9P 406940-85-0P 406940-86-1P 406940-87-2P 406940-88-3P
406940-89-4P 406940-90-7P 406940-91-8P 406940-92-9P 406940-93-0P
406940-94-1P 406940-95-2P 406940-96-3P 406940-97-4P 406940-98-5P
406940-99-6P 406941-00-2P 406941-01-3P 406941-02-4P 406941-03-5P
406941-04-6P 406941-05-7P 406941-06-8P 406941-07-9P 406941-08-0P
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406941-14-8P 406941-15-9P 406941-16-0P 406941-17-1P 406941-18-2P
406941-19-3P 406941-20-6P 406941-21-7P 406941-22-8P 406941-23-9P
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406941-35-3P 406941-37-5P 406941-38-6P 406941-40-0P 406941-42-2P
406941-44-4P 406941-46-6P 406941-48-8P 406941-51-3P 406941-53-5P
406941-54-6P 406941-55-7P 406941-56-8P 406941-57-9P 406941-58-0P
406941-59-1P 406941-60-4P 406941-61-5P **406941-62-6P**
406941-63-7P 406941-64-8P 406941-65-9P 406941-66-0P 406941-67-1P
406941-68-2P 406941-72-8P 406941-73-9P 406941-74-0P 406941-75-1P
406941-76-2P 406941-77-3P 406941-79-5P 406941-80-8P 406941-81-9P
406941-82-0P 406941-85-3P 406941-86-4P 406941-88-6P 406941-90-0P
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406941-98-8P 406941-99-9P 406942-00-5P 406942-02-7P 406942-03-8P
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406942-37-8P 406942-38-9P 406942-40-3P 406942-41-4P 406942-42-5P
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406942-48-1P 406942-49-2P 406942-50-5P 406942-51-6P 406942-52-7P
406942-53-8P 406942-54-9P 406942-57-2P 406942-58-3P 406942-61-8P
406942-62-9P 406942-64-1P 406942-65-2P 406942-66-3P 406942-67-4P
406942-69-6P 406942-70-9P 406942-71-0P 406942-73-2P 406942-74-3P
406942-75-4P 406942-76-5P 406942-77-6P 406942-78-7P 406942-79-8P
406942-80-1P 406942-81-2P 406942-83-4P 406942-85-6P 406942-88-9P
406942-89-0P 406942-90-3P 406942-91-4P 406942-92-5P 406942-93-6P
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406943-23-5P 406943-24-6P 406943-26-8P 406943-27-9P 406943-28-0P
406943-30-4P 406943-31-5P 406943-32-6P 406943-34-8P 406943-35-9P
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406943-52-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzimidazolone **antiviral** agents)

IT 406943-54-2P 406943-57-5P 406943-58-6P 406943-59-7P 406943-60-0P
406943-61-1P 406943-62-2P 406943-63-3P 406943-64-4P 406943-65-5P
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406943-73-5P 406943-74-6P 406943-75-7P 406943-76-8P 406943-77-9P
406943-78-0P 406943-79-1P 406943-80-4P 406943-81-5P 406943-82-6P
406943-83-7P 406943-88-2P 406943-90-6P 406943-92-8P 406943-93-9P
406943-94-0P 406943-95-1P 406943-96-2P 406943-98-4P 406943-99-5P
406944-00-1P 406944-01-2P 406944-02-3P 406944-03-4P 406944-04-5P
406944-05-6P 406944-06-7P 406944-08-9P 406944-09-0P 406944-10-3P
406944-11-4P 406944-13-6P 406944-14-7P 406944-15-8P 406944-16-9P
406944-17-0P 406944-18-1P 406944-19-2P 406944-20-5P 406944-21-6P
406944-24-9P 406944-25-0P 406944-26-1P 406944-27-2P 406944-28-3P
406944-29-4P 406944-30-7P 406944-32-9P 406944-33-0P 406944-34-1P
406944-35-2P 406944-37-4P 406944-38-5P 406944-39-6P 406944-40-9P
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406944-56-7P 406944-57-8P 406944-58-9P 406944-60-3P 406944-61-4P
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406944-78-3P 406944-80-7P 406944-81-8P 406944-82-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzimidazolone **antiviral** agents)

IT 60-24-2, Mercaptoethanol 66-22-8, Uracil, reactions 70-11-1, 2-Bromoacetophenone 78-94-4, Methyl vinyl ketone, reactions 79-44-7, n,N-Dimethylcarbamoyl chloride 96-32-2, Methyl bromoacetate 98-09-9, Benzenesulfonyl chloride 105-36-2, Ethyl bromoacetate 107-13-1, Acrylonitrile, reactions 107-82-4, 1-Bromo-3-methylbutane 107-85-7, 3-Methylbutylamine 108-00-9, N,N-Dimethylethylenediamine 109-01-3, N-Methylpiperazine 109-83-1, N-Methylaminoethanol 109-85-3, 2-Methoxyethylamine 109-90-0, Ethyl isocyanate 141-97-9, Ethyl acetoacetate 156-87-6 288-13-1, Pyrazole 364-74-9, 2,5-Difluoronitrobenzene 462-72-6, 1-Bromo-4-fluorobutane 535-11-5, Ethyl 2-bromopropionate 542-81-4 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene 626-67-5, N-Methylpiperidine 682-30-4 683-60-3, Sodium isopropoxide 836-42-0, 4-Benzyloxybenzyl chloride 870-63-3, 1-Bromo-3-methyl-2-butene 939-80-0, 4-Chloro-3-nitrobenzonitrile 1072-52-2, 2-(Aziridin-1-yl)ethanol 1120-71-4, [1,2]Oxathiolane 2,2-dioxide 1129-28-8, Methyl 3-(bromomethyl)benzoate 1493-27-2, 2-Fluoronitrobenzene 1632-83-3, N-Methylbenzimidazole 1703-46-4, 4-(N,N-Dimethylamino)benzyl alcohol 1849-01-0, 1-Methyl-2-benzimidazolone 2417-72-3, Methyl 4-(bromomethyl)benzoate 2417-73-4, Methyl 2-(bromomethyl)benzoate 3680-02-2, Methyl vinyl sulfone 4104-45-4, 3-(Methylthio)propylamine 4584-46-7, N-(2-Chloroethyl)dimethylamine hydrochloride 4753-59-7, 4-Bromobutyl acetate 4856-97-7, 2-(Hydroxymethyl)benzimidazole 4857-04-9, 2-(Chloromethyl)benzimidazole 5292-43-3, tert-Butyl bromoacetate 5332-06-9, 4-Bromobutyronitrile 5407-04-5, N-(3-Chloropropyl)dimethylamine hydrochloride 5414-21-1, 5-Bromovaleronitrile 5465-65-6 5978-08-5 6232-88-8, 4-Bromomethylbenzoic acid 7250-67-1, N-(2-Chloroethyl)pyrrolidine hydrochloride 10045-45-1, 1-Ethyl-1,3-dihydrobenzimidazol-2-one 10147-37-2, Isopropylsulfonyl chloride 13220-33-2, 1-Methyl-3-hydroxypyrrolidine 13325-10-5, 1-Amino-4-butanol 13795-73-8, Di-tert-butyl aspartate 14813-85-5 18645-88-0, 3-Fluorobenzene-1,2-diamine 19810-31-2, Benzyloxyacetyl

chloride 20662-53-7 20780-53-4 27988-97-2, Tetrazole 32213-95-9, Dimethyl L-aspartate hydrochloride 32754-99-7, 4-Aminobutyronitrile 40517-43-9, 1-(Methanesulfonyl)-4-(chloromethyl)benzene 41120-23-4 52099-72-6, 1-Isopropenyl-2-benzimidazolone 57683-71-3, 2-Carbomethoxybenzenesulfonamide 76179-40-3, 2-Amino-4,5-difluoroaniline 142649-86-3 144655-76-5 161468-47-9 161468-55-9 222978-03-2, 2-Fluoro-4-(bromomethyl)benzonitrile 406945-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzimidazolone **antiviral** agents)

IT 4113-97-7P 4926-55-0P 23937-68-0P 25238-55-5P 35562-81-3P
35681-40-4P 43215-12-9P 51138-16-0P 56436-25-0P 56636-93-2P
56636-95-4P 64266-27-9P 69449-20-3P 78156-03-3P 87120-81-8P
104189-83-5P 125460-21-1P 256366-08-2P 257869-92-4P 346694-26-6P
347355-52-6P 380543-66-8P 380604-60-4P 380604-61-5P 380604-62-6P
380604-63-7P 380604-64-8P 380604-65-9P 380604-66-0P 380604-67-1P
380604-70-6P 380604-71-7P 380604-72-8P 380604-73-9P 380604-83-1P
380604-84-2P 380605-11-8P 406944-83-0P 406944-84-1P 406944-85-2P
406944-86-3P 406944-87-4P 406944-88-5P 406944-89-6P 406944-90-9P
406944-91-0P 406944-92-1P 406944-93-2P 406944-94-3P 406944-95-4P
406944-96-5P 406944-97-6P 406944-98-7P 406944-99-8P 406945-00-4P
406945-01-5P 406945-02-6P 406945-03-7P 406945-04-8P 406945-05-9P
406945-06-0P 406945-10-6P 406945-11-7P 406945-12-8P 406945-13-9P
406945-14-0P 406945-15-1P 406945-16-2P 406945-17-3P 406945-18-4P
406945-19-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of benzimidazolone **antiviral** agents)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Meanwell; J Org Chem 1995, V60(6), P1565 CAPLUS

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	57.23	436.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.54	-11.77

FILE 'CAPLUS' ENTERED AT 10:05:00 ON 21 JAN 2004

FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d his

     (FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

     FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004
L1                STRUCTURE UPLOADED
L2              0 S L1 EXA SAM
L3              0 S L1 FAM SAM
L4             50 S L1 SSS SAM

     FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
L5             10 S L4

     FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004
L6           4073 S L1 SSS FULL
L7           3719 S HIV OR RETROVIRAL OR RETROVIRUS
L8           2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

     FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004
L9          70667 S HIV OR RETROVIRAL OR RETROVIRUS
L10         31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV
L11           636 S L6
L12             9 S L11 AND L9

     FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004
L13             1 S 188839-16-9/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004

     FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004
L14             1 S 457949-18-7/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004
L15             5 S L11 AND L10
L16             2 S L15 NOT L12

     FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004
L17             1 S 174398-05-1/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004

     FILE 'REGISTRY' ENTERED AT 09:51:38 ON 21 JAN 2004
L18             1 S 26148-35-6/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:54:26 ON 21 JAN 2004
                  E ANTIVIRAL
L19         41468 S E3-E9
L20            21 S L19 AND L11
L21            15 S L20 NOT L12
L22            13 S L21 NOT L16
```

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     FILE 'CAPLUS' ENTERED AT 10:05:00 ON 21 JAN 2004

=> d his

     (FILE 'HOME' ENTERED AT 09:19:58 ON 21 JAN 2004)

     FILE 'REGISTRY' ENTERED AT 09:20:03 ON 21 JAN 2004
L1             STRUCTURE UPLOADED
L2           0 S L1 EXA SAM
L3           0 S L1 FAM SAM
L4          50 S L1 SSS SAM

     FILE 'CAPLUS' ENTERED AT 09:27:43 ON 21 JAN 2004
L5          10 S L4

     FILE 'REGISTRY' ENTERED AT 09:31:51 ON 21 JAN 2004
L6        4073 S L1 SSS FULL
L7        3719 S HIV OR RETROVIRAL OR RETROVIRUS
L8        2422 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV

     FILE 'CAPLUS' ENTERED AT 09:34:16 ON 21 JAN 2004
L9       70667 S HIV OR RETROVIRAL OR RETROVIRUS
L10      31317 S HERPES OR HERPETIC OR HSV OR HCMV OR CMV OR HHV
L11        636 S L6
L12          9 S L11 AND L9

     FILE 'REGISTRY' ENTERED AT 09:41:14 ON 21 JAN 2004
L13          1 S 188839-16-9/RN
               SET NOTICE 1 DISPLAY
               SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:42:34 ON 21 JAN 2004

     FILE 'REGISTRY' ENTERED AT 09:47:14 ON 21 JAN 2004
L14          1 S 457949-18-7/RN
               SET NOTICE 1 DISPLAY
               SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:48:05 ON 21 JAN 2004
L15          5 S L11 AND L10
L16          2 S L15 NOT L12

     FILE 'REGISTRY' ENTERED AT 09:49:33 ON 21 JAN 2004
L17          1 S 174398-05-1/RN
               SET NOTICE 1 DISPLAY
               SET NOTICE LOGIN DISPLAY
               SET NOTICE 1 DISPLAY
               SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:50:25 ON 21 JAN 2004

     FILE 'REGISTRY' ENTERED AT 09:51:38 ON 21 JAN 2004
L18          1 S 26148-35-6/RN
               SET NOTICE 1 DISPLAY
               SET NOTICE LOGIN DISPLAY

     FILE 'CAPLUS' ENTERED AT 09:54:26 ON 21 JAN 2004
               E ANTIVIRAL
L19      41468 S E3-E9
L20         21 S L19 AND L11
L21         15 S L20 NOT L12
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L22           13 S L21 NOT L16

     FILE 'CAPLUS' ENTERED AT 10:05:00 ON 21 JAN 2004

=>

---Logging off of STN---


=>
Executing the logoff script...


=> LOG Y

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       7.01     443.72

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00     -11.77

STN INTERNATIONAL LOGOFF AT 10:14:26 ON 21 JAN 2004
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